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> Barb O'Bryen Technical Info. Specialist

CM1 12014 Tel: 308-4291

Point of Contact: **Toby Port** Technical Info. Specialist CM1 1E01 TEL: 308-3534

308-4488 John Dantzman Susan J iley Jan Delaval 308-4498 Mary Hale 308-4258 305-4053 **Edward Hart** 305-9203 Barb O'Bryen 308-4291 **Toby Port** 308-3534 David . reiber 308-4292 Beverly Shears 308-4994 Paula Sheppard 308-4499 Alex Waclawiw 308-4491 Mona Smith 308-3278

Compliment or Complaint, contact:

Stephanie Publicker Chief, Information Branch - STIC Phone: 308-4740

Arti Shah Division Chief - Biotech/Chem Division - STIC

Phone: 308-4259

	19305	,		TMENT OF COMMERCE
ob s	EARCH REQUE	ST FORM		
Requestor's Name: GCAUIII		Serial Number:	14:56	51.
Date:	Phone: 305	2446 Rm	Art Unit: 1()	-MI
Search Topic: Please write a detailed statement of search that may have a special meaning. Give exa a copy of the sequence. You may include	imples or relevant citations, au	thors keywords, etc.,	natter to be searched.	Define any terms tees, please attach
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		J.a.		
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Total time: Number of Searches: Number of Databases:		N.A. Sequence A.A. Sequence Structure		Geninfo SDC DARC/Ouestel

Bibliographic

Other

Wei & Y?/au	Ahmad, I
May hew, E	Janoff, A

16. A compound having the formula R¹-Y¹-CHZ¹/CH(NY²Y³)-CH₂/Z², wherein:

R¹ is a straight-chained alkyl, alkenyl or alkynyl group having from 5 to 19 carbon atoms in the aliphatic chain;

 Y^1 is -CH=CH-, -C=C- or -CH(OH)CH(OH)-;

- Z^1 is OH or a phosphorylcholine attachment-inhibiting group selected from the group consisting of $-X^1$, $-OX^1$, $-X^2X^3$ and $-OX^2X^3$;
- Y² is H, a phenyl group, an alkyl-substituted phenyl group having from 1 to about 6 carbons in the alkyl chain, or an alkyl chain having from 1 to 10 carbons;
- Y^3 is H or a group having the formula $-C(O)R^2$ or $-S(O)_2R^2$;
- R² is a straight-chained alkyl moiety selected from the group consisting of -(CH₂)₃CH₃, -(CH₂)₅CH₃, -(CH₂)₇CH₃ and -(CH₂)₉CH₃, an alkenyl group group having from 1 to 23 carbon atoms in the aliphatic chain and an alkynyl group having from 1 to 23 carbon atoms in the aliphatic chain;

Z² is OH or a phosphorylcholine attachment-inhibiting group selected from the group consisting of -X¹, -OX¹, -X²X³ and -OX²X³;

- X¹ is selected from the group consisting of -C(O)H, -CO₂H, CH₃(C(CH₃)₃)₂, Si(C(CH₃)₃)₃, Si(PO₄)₂C(CH₃)₃, a phenyl group, an alkyl-substituted phenyl group having from 1 to 6 carbons in the alkyl chain, an alkyl chain having from 1 to 6 carbons, an amino group, a fluorine, a chlorine, and a group having the formula C(R³R⁴)OH:
- X² is selected from the group consisting of CH₂-, C(CH₃)₂-, Si(PO₄)₂-, Si(CH₃)₂-, Si(CH₃)₂-
- X³ is selected from the group consisting of -C(O)H, -CO₂H, -CH₃, -C(CH₃)₃, -Si(CH₃)₃, -Si(CH₃)₃, -Si(C(CH₃)₃)₂, -Si(C(CH₃)₃)₃, -Si(PO₄)₂C(CH₃)₃, a phenyl group, an alkyl-substituted phenyl group having from 1 to 6 carbons in the alkyl chain, an alkyl chain having from 1 to 6 carbons, an amino moiety, a chlorine, a fluorine, or a group having the formula C(R³R⁴)OH, wherein each of R³ and R⁴ is independently an alkyl chain having from 1 to 6 carbons, a phenyl group or an alkyl-substituted phenyl group having from 1 to 6 carbons in the alkyl chain;

carbon

carbon

carbon

carbon

carbon

carbon

ch3

ch3

ch3

ch3

ch3

wherein when Z² is an amino group, R² is an aliphatic chain having from 1 to 9 or from 19 to 23 carbon atoms in the aliphatic chain.

- 17. The compound of claim 16, wherein R² is an alkyl chain.
- 18. The compound of claim 16, wherein R¹ is CH₃(CH₂)₁₂-.
- 19. The compound of claim 16, wherein Y¹ is -CH=CH-.
- 20. The compound of claim 16, wherein Y² is H.
- 21. The compound of claim 16, wherein Y^3 is $-C(O)R^2$.
- 22. The compound of claim 16, wherein Z¹ is OH.
- 23. The compound of claim 22, wherein Z^2 is a group having the formula $-X^2X^3$ or $O-X^2X^3$.
- 24. The compound of claim 23, wherein Z² is -OC(O)CH₃, -OC(O)CH₂CH₂CH₃, -OC(O)CH(CH₃)CH₃, or -OSi(CH₃)₂C(CH₃)₃.
- 25. The compound of claim 24, wherein Z² is -OSi(CH₃)₂C(CH₃)₃.
- 26. The compound of claim 22, wherein Z^2 is a group having the formula $-X^1$ or OX^1 .
- 27. The compound of claim 16 having the formula CH₃(CH₂)₁₂-CH=CH₂CH₂Z¹-CH(NHY³)-CH₂-Z².

carbon a valence of 5

- 28. The compound of claim 27, wherein Z^1 is OH and Y^3 is a group having the formula $-C(O)R^2$.
- 29. The compound of claim 28, wherein Y³ is -C(O)(CH₂)₄CH₃.
- 30. The compound of claim 27, wherein Z² is -OSi(CH₃)₂C(CH₃)₃, -OSi(PO₄)₂C(CH₃)₃, -C(O)CH₃ or -OC(O)CH₂CH₂CH₃.
- 31. A pharmaceutical composition comprising the compound of claim 16.
- 32. A liposome having a bilayer comprising a lipid component, said lipid component comprising at least about 5 mole percent of the compound of claim 16.



Fig.

APPROVED O.G. FIG

DRAFTSMAN

₩

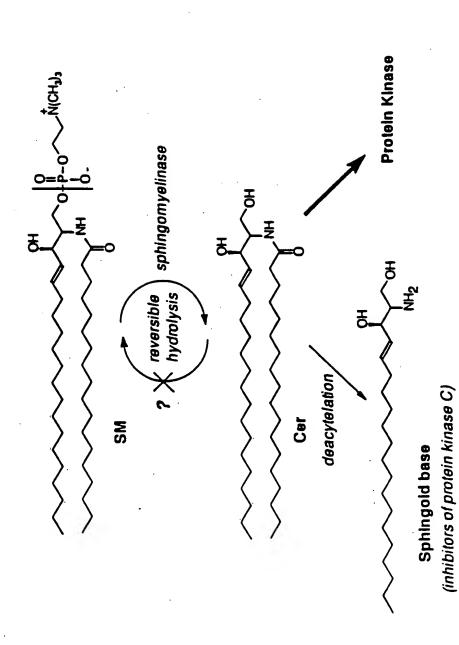


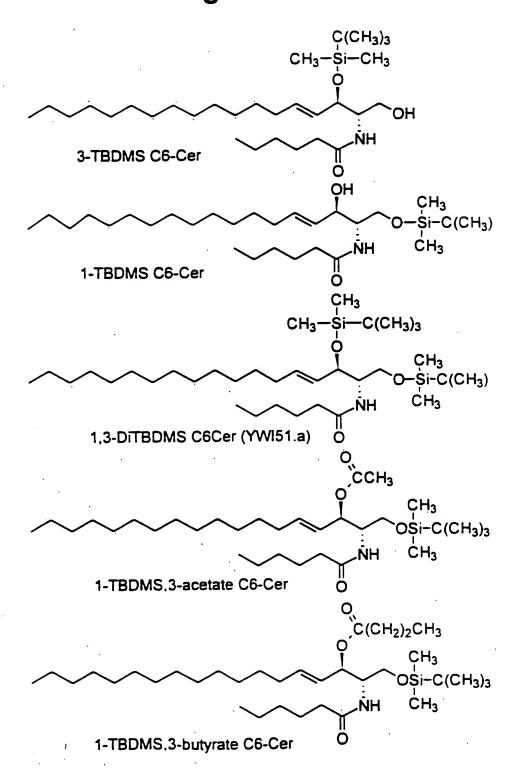
Fig. 2a

Type III Cer-1-TBDMS

APPROVED C.G. FIG.
BY CLASS SUBC

C6 Cer-1-TBDMS

Fig. 2b



APPROVED O.G. FIG.
BY GLASS SUBCLASS
DRAFTSMAN



Fig. 2c

4,5-Diol C6-Cer

0.G. FIG.	CLASS SUBCLASS	78
APPROVED O.G. FI	8	DRAFTSMAN

Fig. 2d

N-Hexyl Sphingosine (or N-C6 Sphingosine)

N-C8 Sphingosine

N-C10 Sphingosine

=> file reg; d stat que 117

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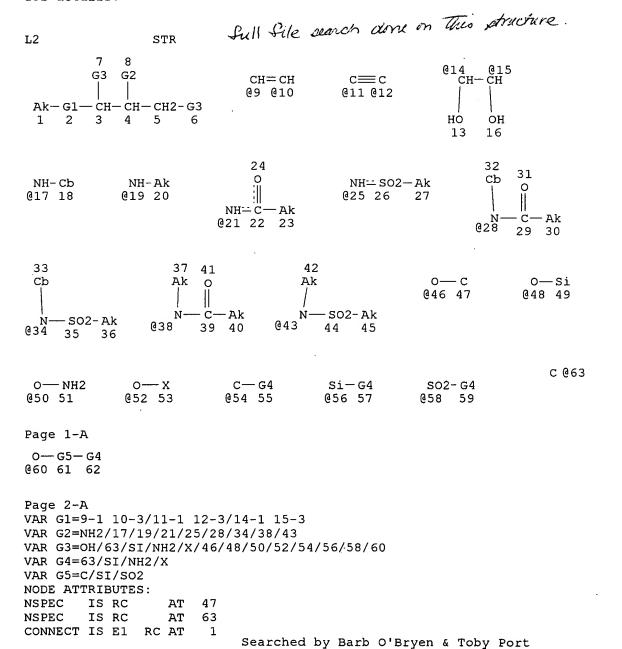
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STRUCTURE FILE UPDATES: 6 JUL 2000 HIGHEST RN 275353-73-6 DICTIONARY FILE UPDATES: 6 JUL 2000 HIGHEST RN 275353-73-6

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Structure search limits have been increased. See HELP SLIMIT for details.



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CONNECT IS E1 RC AT
                    20
CONNECT IS E1 RC AT
CONNECT IS E1 RC AT
                    27
CONNECT IS E1 RC AT
                    30
CONNECT IS E1 RC AT
                   36
CONNECT IS E1 RC AT
                   37
CONNECT IS E1 RC AT
                   40
CONNECT IS E1 RC AT
                   42
CONNECT IS E1 RC AT 45
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       IS MCY UNS AT
GGCAT
       IS MCY UNS AT
GGCAT
GGCAT
       IS MCY UNS AT 33
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E6 C AT
       IS E6 C AT
ECOUNT
ECOUNT
      IS E6 C AT
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GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 63

STEREO ATTRIBUTES: NONE L3 STR

- this structure NOTed out of full file answer set.

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 6

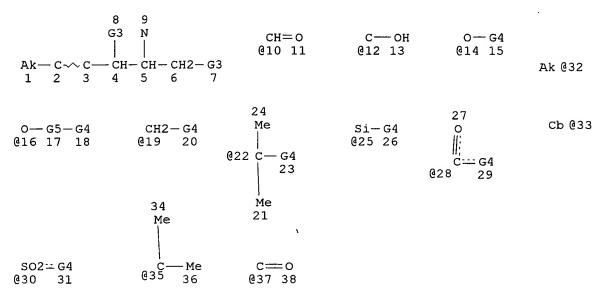
STEREO ATTRIBUTES: NONE

JA COS CER ETT

L7 STR

983 SEA FILE=REGISTRY SSS FUL L2 NOT L3 STR subfile planch done on this structure, shown on page 3

ZI + ZZ more specifically defined.



VAR G3=OH/10/COOH/32/SI/33/NH2/X/12/14/16/19/22/25/28/30
VAR G4=10/COOH/32/SI/33/NH2/X/12
VAR G5=CH2/35/SI/37/SO2
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 32
DEFAULT MLEVEL IS ATOM
GGCAT IS LIN AT 1
GGCAT IS MCY UNS AT 33
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M5-X19 C AT 1
ECOUNT IS E6 C AT 33

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE

VAR G1=11/SO2 NODE ATTRIBUTES: CONNECT IS E1 RC AT 10 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L17 3 SEA FILE=REGISTRY SUB=L10 SSS FUL L15

100.0% PROCESSED 3 ITERATIONS 3 ANSWERS

SEARCH TIME: 00.00.01

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L2		STR	
L3		STR	
L4	983	SEA	FILE=REGISTRY SSS FUL L2 NOT L3
L7		STR	
L10	650	SEA	FILE=REGISTRY SUB=L4 SSS FUL L7
L15		STR	
L17	3	SEA	FILE=REGISTRY SUB=L10 SSS FUL L15
L18	1	SEA	FILE=CAPLUS ABB=ON PLU=ON L17

=> d ibib abs hitstr 118 1; file caold; d que nos 119

L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2000 ACS ACCESSION NUMBER: 2000:199315 CAPLUS

DOCUMENT NUMBER: 132:236933

TITLE: Preparation of sphingomyelinase-inhibiting ceramide

analogs

INVENTOR(S): Kiso, Makoto; Ishida, Shuji

PATENT ASSIGNEE(S): Ohtsuka Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 2000086601 A2 20000328 JP 1998-251197 19980904

OTHER SOURCE(S): MARPAT 132:236933

GΙ

RNH CH CH CH CH CH
$$\frac{1}{2}$$
 CH CH $\frac{1}{2}$ CH $\frac{1}{2}$

AB Ceramide analogs I [R = H, (halo)alkoxycarbonyl; n = 0-22] or their salts are prepd. I show sphingomyelinase inhibition, ceramide glucosylation promotion, sphingosine acyltransferase inhibition, ceramide antagonism, etc., and are useful for treatment of dementia, memory disturbance, inflammation, etc. (no data). (2S,3R,4E)-2-acetylamino-1-azido-4-octadecen-3-ol (prepn. given) was treated with PPh3 in C6H6/H2O at 55.degree. for 3 h to give 75% I (R = H, n = 0).

RN 262288-84-6 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-1-(aminomethyl)-2-hydroxy-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

$$H_2N$$
 S
 R
 E
 (CH_2)
 12
 Me

RN 262288-85-7 CAPLUS

CN Octadecanamide, N-[(1S, 2R, 3E)-1-(aminomethyl)-2-hydroxy-3-heptadecenyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 262288-86-8 CAPLUS

CN Tetracosanamide, N-[(1S,2R,3E)-1-(aminomethyl)-2-hydroxy-3-heptadecenyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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L2		STR	
L3		STR	
L4	983	SEA	FILE=REGISTRY SSS FUL L2 NOT L3
L7		STR	
L10	650	SEA	FILE=REGISTRY SUB=L4 SSS FUL L7
L15		STR	
L17	3	SEA	FILE=REGISTRY SUB=L10 SSS FUL L15
L19	0	SEA	FILE=CAOLD ABB=ON PLU=ON L17

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NSPEC

NSPEC

IS RC

IS RC

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47

63

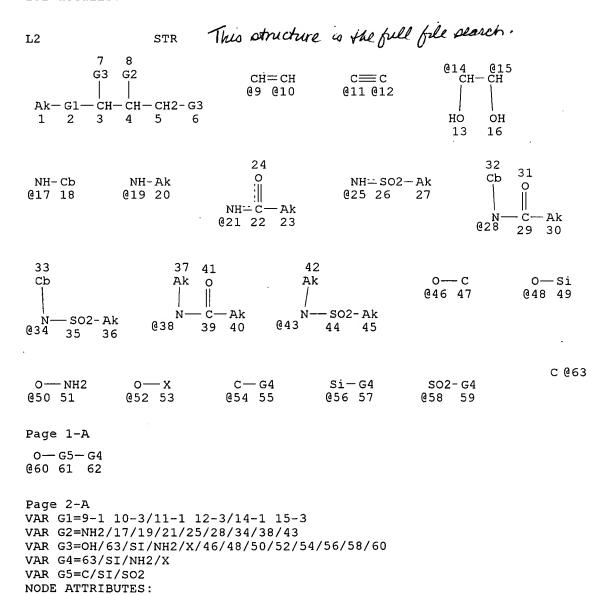
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```
CONNECT IS E1 RC AT
                      1
CONNECT IS E1 RC AT
                     20
CONNECT IS E1
                     23
             RC AT
CONNECT IS E1
                     27
             RC AT
CONNECT IS E1 RC AT
                     30
CONNECT IS E1 RC AT
                     36
                     37
CONNECT IS E1 RC AT
                     40
CONNECT IS E1 RC AT
                     42
CONNECT IS E1 RC AT
                    45
CONNECT IS E1 RC AT
DEFAULT MLEVEL IS ATOM
GGCAT
       IS MCY UNS AT
                        18
       IS MCY
                        32
GGCAT
              UNS
                    AT
                        33
       IS MCY UNS AT
GGCAT
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E6 C AT
                    18
ECOUNT
       IS E6 C AT
                    32
                    33
ECOUNT IS E6 C AT
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GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 63

STEREO ATTRIBUTES: NONE
L3 STR Thus structure is NOTed out of full file search results.

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE

T.4

983 SEA FILE=REGISTRY SSS FUL L2 NOT L3

L7

Subfile slaich done on this structure, shown on page 9.

ZI + Zz more specifically defined

1

ţ

8 9 G3 N CH = OС---ОН o— G4 @14 15 010 11 @12 13 $Ak-C \sim C-CH-CH-CH2-G3$ Ak @32 2 3 4 5 6 24 27 Me Cb @33 0 - G5 - G4CH2-G4 si-G40 @16 17 18 @19 20 @25 26 @22 C-G4 C--- G4 23 @28 29 Me 34 21 Me SO2=G4 c=0@37 38 @30 31

Kishore

09/429,694

VAR G3=OH/10/COOH/32/SI/33/NH2/X/12/14/16/19/22/25/28/30 VAR G4=10/COOH/32/SI/33/NH2/X/12 VAR G5=CH2/35/SI/37/SO2 NODE ATTRIBUTES: CONNECT IS E1 RC AT 32 DEFAULT MLEVEL IS ATOM GGCAT IS LIN AT GGCAT IS MCY UNS AT 33 DEFAULT ECLEVEL IS LIMITED ECOUNT IS M5-X19 C AT ECOUNT IS E6 C AT 33

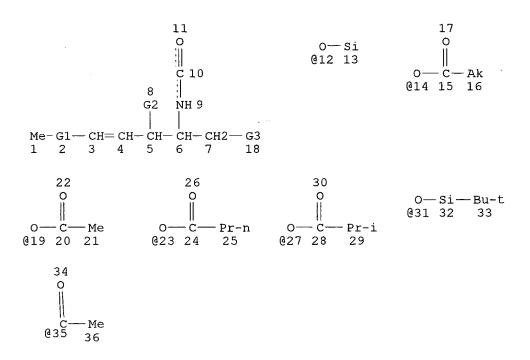
GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE

L10 L28

650 SEA FILE=REGISTRY SUB=L4 SSS FUL L7 L10 has form many answers, 20 STR

atructure 128 further newows the answer sub-Definitions from claims 18,19,20,21,22,24,25+30 are used to further define the structure of 628.



REP G1=(12-14) CH2
VAR G2=OH/12/14
VAR G3=19/23/27/31/35
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DEFAULT MLEVEL IS ATOM
GGCAT IS LIN LOC AT 16
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 36 STEREO ATTRIBUTES: NONE

L31 46 SEA FILE=REGISTRY SUB=L10 SSS FUL L28

100.0% PROCESSED 150 ITERATIONS 46 ANSWERS

SEARCH TIME: 00.00.02

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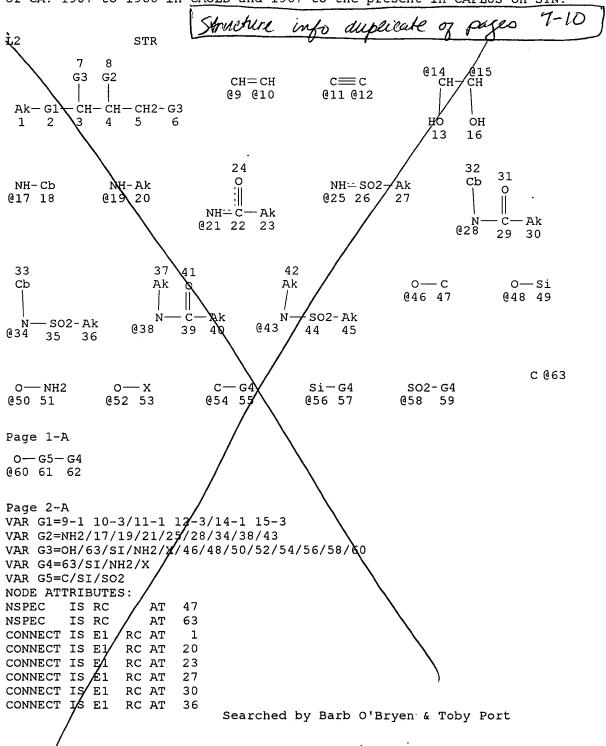
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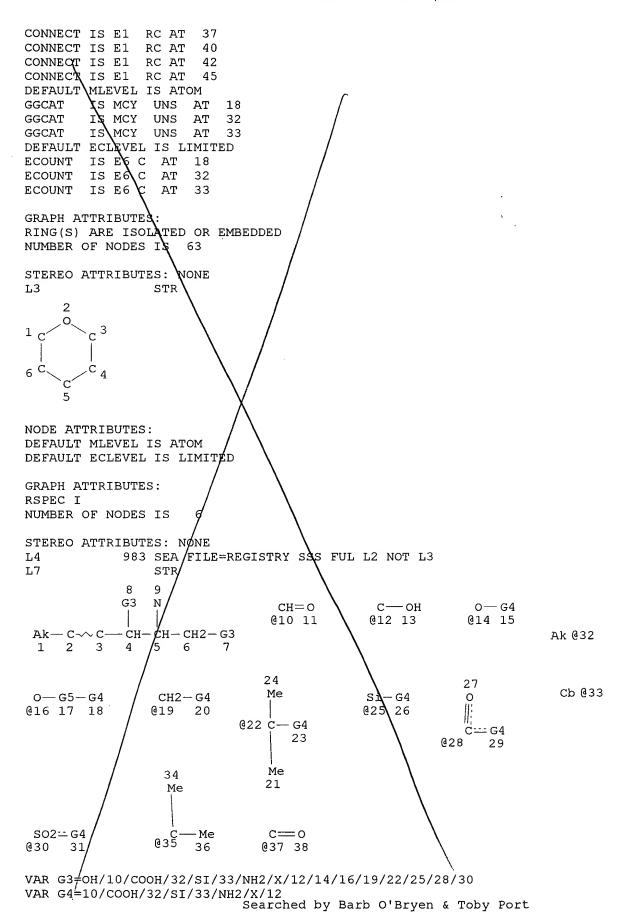
FILE COVERS 1967 - 7 Jul 2000 VOL 133 ISS 2
FILE LAST UPDATED: 6 Jul 2000 (20000706/ED)
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```
VAR G5=CH2/35/SI/37/SO2
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 32
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GGCAT
        IS MCY UNS AT
DEFAULT ECLEVEL IS LIMITED
ECOUNT)
      IS M5-X19 C AT
ECOUNT\
       IS E6 C AT
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OF EMBEDDED
NUMBER OF NODES IS 38
STEREO ATTRIBUTES: NONE
L10
           650 SEA /FILE=REGISTRY SUB=L4 SSS FUL L7
L28
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                   0
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                                     o-si
                                    @12 13
                   C 10
                                                 0-C-Ak
                                                 @14 15 16
               'G2
                   NH 9
Me-G1-CH=CM-
               \CH- CH- CH2- G3
                   6 7
 1 2
        3
                           18
    22
                    26
                                    30
    0
                                     0
                                                 o-si-Bu-t
                                                 @31 32 33
 o---c-
                    - C-
                        -Pr-n
                                 o--- c-
                                        -Pr-i
                                @27 28
@19 20
                @2\3 24
                        25
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VAR $3=19/23/27/31/35
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 16
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GGCAT IS LIN LOC AT
DEFAULT ECLEVEL IS LIMITED
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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 36
STEREO ATTRIBUTES: NONE
L31
             46 SEA FILE=REGISTRY SUB=L10 SSS FUL L28
L32
             72 SEA FILE=CAPLUS ABB=ON PLU=ON L31
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=> d ibib abs hitstr 132 1-72; file caold; dque nos 133

L32 ANSWER 1 OF 72 CAPLUS COPYRIGHT 2000 ACS ACCESSION NUMBER: 2000:128525 CAPLUS

DOCUMENT NUMBER: 132:293951

TITLE: A chemoenzymatic access to D- and L-sphingosines

employing hydroxynitrile lyases

AUTHOR(S): Johnson, Dean V.; Felfer, Ulfried; Griengl, Herfried CORPORATE SOURCE: Spezialforschungsbereich Biokatalyse, Institut fur

Organische Chemie der Technischen Universitat Graz,

Graz, A-8010, Austria

SOURCE: Tetrahedron (2000), 56(5), 781-790

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

AB A chemoenzymic access to D- or L-sphingosines is presented comprising of a total synthesis of the L-threo-isomer and formal syntheses of the other three isomers. Key to the development of a general synthetic strategy has been the use of enantio-complementary hydroxynitrile lyases (Hnls) to yield an enantiomeric pair of starting materials. The (S)-Hnl from Hevea brasiliensis has been used to prep. L-threo-sphingosine in 14 steps and an overall 12% yield. Application of the (R)-Hnl from Prunus amygdalus formally allows synthesis of D-threo- and D-erythro-sphingosines.

IT 78779-96-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (chemoenzymic access to D- and L-sphingosines employing hydroxymitrile
 lyases)

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

REFERENCE COUNT:

53

REFERENCE(S):

INVENTOR(S):

- (1) Albrecht, J; Biotechnol Appl Biochem 1993, V17, P191 CAPLUS
- (2) Baker, R; J Chem Soc, Perkin Trans 1 1989, P190 CAPLUS
- (3) Borek, C; Proc Natl Acad Sci USA 1991, V88, P1953 CAPLUS
- (4) Brussee, J; Tetrahedron 1990, V46, P979 CAPLUS
- (5) Brussee, J; Tetrahedron 1990, V46, P979 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1999:787651 CAPLUS

DOCUMENT NUMBER: 132:18776

TITLE: Preparation of fat emulsions which contains the

ceramide derivatives as cancer metastasis inhibitors Mizushima, Hiroshi; Igarashi, Toshisato; Mizushima,

Noboru; Takenaga, Mitsuko; Morisawa, Yoshitomi;

Nakayama, Toshiaki

PATENT ASSIGNEE(S): LTT Inst. Co., Ltd., Japan; Asahi Glass Co., Ltd.

SOURCE:

Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE ____ _____ -----_____ A2 19991214 JP 11343249 JP 1998-150128 19980529

OTHER SOURCE(S):

MARPAT 132:18776

Fat emulsions which contains the ceramide derivs. (Markush's structure given) are claimed as cancer metastasis inhibitors. The antimetastatic effect of the ceramide derivs. was tested in mice.

IT 2482-37-3P

> RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(CeRa-03; prepn. of fat emulsions which contains the ceramide derivs. as cancer metastasis inhibitors)

2482-37-3 CAPLUS RN

Acetamide, N-[(1S, 2R, 3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-CN heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 3 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER:

1999:712892 CAPLUS

DOCUMENT NUMBER:

132:212571

TITLE:

Lipid microsphere preparation of a lipophilic ceramide derivative suppressed the colony formation of murine

experimental metastasis

AUTHOR (S):

Takenaga, Mitsuko; Igarashi, Rie; Matsumoto, Kayo; Mizushima, Noboru; Nakayama, Toshiaki; Mizushima,

Yutaka

CORPORATE SOURCE:

The Second Department of the Institute of Medical Science, St. Marianna University School of Medicine,

Kanagawa, 216-8512, Japan

SOURCE:

Drug Delivery Syst. (1999), 14(5), 373-379

CODEN: DDSYEI; ISSN: 0913-5006 Nippon DDS Gakkai Jimukyoku

DOCUMENT TYPE:

Journal Japanese

PUBLISHER: LANGUAGE:

ΔR Ceramide is well known as a regulator of cell apoptosis and cell growth suppression. In this study, we synthesized more lipophilic ceramide derivs. in order to incorporate into lipid microsphere (LM), and their activity was evaluated in vivo. Cera 03, a diacetylated form of

C2-ceramide showed a potent cell growth inhibition and potently induced apoptosis in both U 937 cells and Meth A-T tumor cells in vitro, with a similar potency as cell membrane-permeable C2-ceramide. Diacetylated form of natural type ceramide (Cer), Cera 02, also suppressed the in vitro cell growth with a similar potency as that of Cer. which was much lower than Searched by Barb O'Bryen & Toby Port

Page 16

that of C2-ceramide and Cera 03. LM prepn. of Cera 03 (Lipo-Cera 03, 1 mg/mL) was stable, and inhibited the murine exptl. pulmonary metastasis employed with Meth A-T cells. I.v. injection of lipo-Cera 03 (1 mg/kg of Cera 03) showed over 35% inhibition in the exptl. metastasis model. In while, LM prepn. of Cera 02 (Lipo-Cera 02, 1 mg/mL) was also stable, however, a significant efficacy was not obsd. Therefore, LM emulsion of a ceramide deriv. (Cera 03) has a potential for an anti-metastatic injectable drug, and also would be an useful tool for researching the role of ceramide in vivo.

IT 67113-24-0P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(lipid microsphere prepn. of a lipophilic ceramide deriv. suppressed colony formation of murine exptl. metastasis)

67113-24-0 CAPLUS RN

CN Acetamide, N-[(1R,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3heptadecenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry. Double bond geometry as shown.

L32 ANSWER 4 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1999:672566 CAPLUS

DOCUMENT NUMBER: 131:295576

TITLE: Spisulosine compounds having antitumor activity

Rinehart, Kenneth Lloyd; Fregeau, Nancy Louise; INVENTOR (S): Warwick, Robert Arthur; Garcia Gravalos, Dolores;

Avila, Jesus; Faircloth, Glynn Thomas

The Board of Trustees of the University of Illinois, PATENT ASSIGNEE(S):

USA; Ruffles, Graham, Keith

SOURCE: PCT Int. Appl., 73 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.			KIND DATE				APPLICATION NO. DATE										
	WO 9952521			A1 19991021				WO 1999-GB1091 19990409										
		w:	ΑE,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,
			DE,	DK,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,
			JP,	KΕ,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,
			MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,
			TM,	TR,	TT,	UA,	UG,	US,	UZ,	VN,	YU,	ZA,	ZW,	AM,	ΑZ,	BY,	ΚG,	KΖ,
			MD,	RU,	ТJ,	TM												
		RW:	GH,	GM,	KE,	LS,	MW,	SD,	SL,	SZ,	UG,	ZW,	AT,	BE,	CH,	CY,	DE,	DK,
			ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,
			CI,	CM,	GΑ,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG					
PRIO	PRIORITY APPLN. INFO.: US 1998-58456 19980410																	
AB	Inv	resti	gati	on o	f th	e ac	tivi	ty o	f ex	ts.	of t	he c	lam :	Spis	ula j	poly	nyma	has
	AB Investigation of the activity of exts. of the clam Spisula polynyma has led to antitumor long-chain, straight-chain alkane or alkene compds. which																	

have a 2-amino group and a 3-hydroxy group.

IT 2482-37-3P

RL: BOC (Biological occurrence); PUR (Purification or recovery); SPN (Synthetic preparation); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(spisulosine compds. having antitumor activity)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

REFERENCE COUNT:

7

REFERENCE(S):

(1) Bell, R; US 4816450 A 1989

(2) Biomembrane Inst; EP 0381514 A 1990(3) Biomembrane Inst; WO 9618404 A 1996

(4) Kinkade, J; US 5190876 A 1993

(6) Shallenberger, R; EXPERIENTIA 1974, V30(6), P597

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 5 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1999:476763 CAPLUS

DOCUMENT NUMBER:

131:286282

TITLE:

A short enantiodivergent synthesis of D-erythro and

L-threo sphingosine

AUTHOR(S):

Khiar, Noureddine; Singh, Kamaljit; Garcia, Mercedes;

Martin-Lomas, Manuel

CORPORATE SOURCE:

Grupo de Carbohidratos, Instituto de Investigaciones

Quimicas, C.S.I.C., Seville, 41092, Spain Tetrahedron Lett. (1999), 40(31), 5779-5782

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER:

Elsevier Science Ltd.

DOCUMENT TYPE:

Journal

LANGUAGE:

SOURCE:

English

GΙ

AB A new, short (6 steps) and efficient enantiodivergent route to both D-erythro and L threo-sphingosine I and II [HOCH2CH(NH2)CH(OH)CH=CH(CH2)12 Me] is disclosed. The high diastereoselection (100% de) reached in the creation of the C-3 stereocenter relies on the use of a sulfoxide as chiral controlling agent in the redn. of the common precursor Searched by Barb O'Bryen & Toby Port

(R)-.beta.-keto sulfoxide (III) (R = S(=0)-4-Me-C6H4, X = =0). The desired E-alkene of sphingosines has been constructed by the Schlosser modification of the Wittig reaction between the aldehyde III (R = CHO, X = .alpha.OCH2OMe)(IV) and the phosphonium salt Me(CH2)12PPH3Br. The reported methodol. can easily be extended to the synthesis of a large no. of optically pure syn and anti amino alcs. starting from com. available amino acids.

IT 246245-48-7P 246245-49-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(enantiodivergent synthesis of D-erythro and L-threo sphingosine)

RN 246245-48-7 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-octadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 246245-49-8 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-octadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

REFERENCE COUNT: 28

REFERENCE(S): (1) Arnone, A; J Org Chem 1996, V61, P3375 CAPLUS

(3) Carreno, M; Chem Rev 1995, V95, P1717 CAPLUS

(4) Carreno, M; J Org Chem 1990, V55, P2120 CAPLUS

(5) Dietrich, H; Chemistry Eur J 1999, V5, P320 CAPLUS

(7) Enders, D; Chem Eur J 1995, V1, P382 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 6 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER:

1998:758649 CAPLUS

DOCUMENT NUMBER:

130:66723

TITLE:

Preparation of digalactosyl ceramides and their

intermediates

INVENTOR(S):

Nakahon, Kazutaka Eisai Co., Ltd., Japan

PATENT ASSIGNEE(S): SOURCE:

Jpn. Kokai Tokkyo Koho, 11 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 10310596 A2 19981124 JP 1997-119195 19970509

OTHER SOURCE(S): CASREACT 130:66723; MARPAT 130:66723

GI

Title compds. I [R1 = H; X = OR; wherein R = CH2CH(NHCOR2)CH(OR3)CH:CH(CH2)12Me, CH[CH(CH2OR3)NHCOR2]CH:CH(CH2)12Me; R2 = pentadecanyl, heptadecanyl, 8-heptadecenyl; R3 = H] are prepd. by reaction of halides I (X = halo; R1 = protective group) with ROH (R = same as I; R3 = protective group) and deprotection of I (R1 = protective group; X = OR; wherein CH2CH(NHCOR2)CH(OR3)CH:CH(CH2)12Me, CH[CH(CH2OR3)NHCOR2]CH:CH(CH2)12Me; R3 = protective group). The deprotected I are useful as anticancer agents, immunosuppressants, anti-HIV agents, detoxicants, Gaucher disease inhibitors (no data). .beta.(1.fwdarw.4)-I (R1 = Ac, X = F) (prepn. given) was treated with (2S,3R,4E)-1-O-benzoyl-2-N-palmitoylsphingosine (prepn. given) in CH2Cl2 in the presence of AgClO4, TiCl2, and mol. sieve 4A at 0.degree. for 17 h to give 12% protected digalactosyl ceramide, which was deprotected by MeONa in MeOH-THF at room temp. for 90 min to give 72% the title compd. (II).

II

IT 143517-08-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of digalactosyl ceramides as pharmaceuticals)

RN 143517-08-2 CAPLUS

CN Hexadecanamide, N-[(1S,2R,3E)-1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]me thyl]-2-hydroxy-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

L32 ANSWER 7 OF 72 CAPLUS COPYRIGHT 2000 ACS

1998:85260 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 128:101927

Chemoenzymic synthesis of all four stereoisomers of TITLE:

sphingosine from chlorobenzene: glycosphingolipid

precursors

AUTHOR(S): Nugent, Thomas C.; Hudlicky, Tomas

CORPORATE SOURCE: Dep. Chem., Univ. Florida, Gainesville, FL,

32611-7200, USA

J. Org. Chem. (1998), 63(3), 510-520 SOURCE:

CODEN: JOCEAH; ISSN: 0022-3263

American Chemical Society PUBLISHER:

DOCUMENT TYPE: Journal English LANGUAGE:

OTHER SOURCE(S): CASREACT 128:101927

GT

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Advantageous use of homochiral cyclohexadiene-cis-1,2-diol I,, available AB by means of biocatalytic oxidn. of chlorobenzene with toluene dioxygenase, has enabled the synthesis of all four enantiomerically pure C18-sphingosines II. The four requisite azido alc. diastereomers III were accessed by regioselective opening of stereoisomeric epoxides with either azide or halide ions. The configuration of C4 and C5 in azides III defines the stereochem. of the incipient sphingosine chain, liberated from by the oxidative cleavage of the C1-C6 olefin. For L-threo-sphingosine [(2S,3S)-II], lactol IV generated by this cleavage was converted by periodate oxidn. to azido deoxy L-threose V,, which gave (2S,3S)-II upon Wittig olefination and redn. Similarly, D-erythro-sphingosine [(2S,3R)-II] and L-erythro-sphingosine [(2R,3S)-II] were generated from (4S,5S) - and (4R,5R)-III, resp. The last sphingosine [(2R,3R)-II] was synthesized from the silyl-protected azido alc. VI. Subsequent transformations provided silyl-protected azido deoxy D-threose VII, which upon Wittig olefination and redn. gave D-threo-sphingosine [(2R,3R)-II]. Exptl. and spectral data are provided for all new compds.

IT 201340-32-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (chemoenzymic synthesis of all four sphingosine stereoisomers from chlorobenzene)

RN 201340-32-1 CAPLUS

Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, CN $[S-(R^*,S^*)]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

IT 78779-96-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (chemoenzymic synthesis of all four sphingosine stereoisomers from chlorobenzene)

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

L32 ANSWER 8 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1997:589524 CAPLUS

DOCUMENT NUMBER: 127:234526

TITLE: Improved, gram scale synthesis of N,O,O-triacetyl-

erythro- and threo-C18-sphingosines from serine AUTHOR(S): Dondoni, Alessandro; Perrone, Daniela; Turturici,

Elisa

CORPORATE SOURCE: Laboratorio di Chimica Organica, Dipartimento di

Chimica, Universita, Ferrara, 44100, Italy

SOURCE: J. Chem. Soc., Perkin Trans. 1 (1997), (16), 2389-2393

CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 127:234526

AB A formal total synthesis of all four (E)-C18-sphingosine from serine has been carried out. This involves the thiazole-based homologation of the amino acid into a chiral 3-amino-2,4-dihydroxybutanal and the Wittig olefination with the ylide from the C14 alkyl phosphonium salt. The photoisomerization of the resulting mixt. of Z- and E-alkenes affords the target sphingosine. Thus, N,O,O-triacetyl-D-erythro C18-sphingosine and the L-threo isomer were prepd. in 43-44% overall yield from the N- and O-protected 3-amino-2,4-dihydroxybutanals. The corresponding antipodal L-erythro and D-threo isomers can be prepd. in the same way. Conversion of the above acetyl sphingosines into the free sphingoid bases has been reported in the literature.

IT 2482-37-3P 128387-01-9P 195194-55-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(improved gram scale prepn. of N,O,O-triacetyl-erythro- and threo-C18-sphingosines from serine)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

128387-01-9 CAPLUS RN

Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, CN $[R-[R^*,S^*-(Z)]]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 195194-55-9 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, $[S-(R^*,R^*)]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

CAPLUS COPYRIGHT 2000 ACS L32 ANSWER 9 OF 72

ACCESSION NUMBER: 1996:325160 CAPLUS

DOCUMENT NUMBER: 125:87046

Synthesis of D-erythro-sphingosine from D-glucosamine TITLE: AUTHOR(S): Shinozaki, Katsuo; Mizuno, Kazuhiro; Masaki, Yukio

CORPORATE SOURCE: Gifu Pharmaceutical University, Gifu, 502, Japan

SOURCE: Chem. Pharm. Bull. (1996), 44(5), 927-932

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English GΙ

$$C_{12}H_{25}$$

D-Erythro-Sphingosine I was synthesized from D-glucosamine as a chiral AΒ pool through stereo-inversion of the C(3)-hydroxyl group via an oxidn.-redn. sequence, transformation to the erythro-amino-alc. chiron protected as the oxazolidinone, and elongation of the side chain at the C(6)-position.

IT 2482-37-3P

> RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of erythrosphingosine from glucosamine)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 10 OF 72 CAPLUS COPYRIGHT 2000 ACS

1996:257368 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 125:33996

TITLE: Synthetic studies on sphingolipids. 3. Efficient stereo controlled synthesis of D-erythro-sphingosine

from N-benzoyl-D-glucosamine

AUTHOR (S): Murakami, Teiichi; Hato, Masakatsu

CORPORATE SOURCE: National Institute Materials Chemical Research,

Tsukuba, 305, Japan

J. Chem. Soc., Perkin Trans. 1 (1996), (8), 823-7 SOURCE:

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE:

Journal

English LANGUAGE:

OTHER SOURCE(S): CASREACT 125:33996

Me (CH₂) 11 OH
$$CH_2$$
 OH CH_2 OH III

AB D-Erythro-sphingosine I is synthesized from 2-benzamido-2-deoxy-D-Searched by Barb O'Bryen & Toby Port

glucopyranose (II) in a highly regio- and stereo-controlled manner. The key features in the synthesis involve the efficient conversion of II into the vinyl epoxide III and the subsequent SN2'-type reaction with a Grignard reagent in the presence of CuCN to afford the 1-O,2-N-protected sphingosine 11.

IT 2482-37-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (asym. synthesis of erythrosphingosine from glucosamine)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 11 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1996:215544 CAPLUS

DOCUMENT NUMBER: 125:11289

TITLE: Enantiopure aminotriol from D-isoascorbic acid:

Synthesis of D-threo-C-18-sphingosine

AUTHOR(S): Tuch, Arounarith; Saniere, Michele; Le Merrer, Yves;

Depezay, Jean-Claude

CORPORATE SOURCE: Lab. Chim. Biochim., Pharmacologiques Toxicologiques,

Univ. Rene Descartes, Paris, 75270, Fr.

SOURCE: Tetrahedron: Asymmetry (1996), 7(3), 897-906

CODEN: TASYE3; ISSN: 0957-4166

DOCUMENT TYPE: Journal

LANGUAGE: English

OH H27C13 OH NH2 I

AB Enantiopure suitably N,O-protected aminotriol has been prepd. from D-isoascorbic acid. The utility of this homochiral building block in the synthesis of D-threosphingosine I is described via a Wittig reaction on a N,O-protected .beta.-amino-.alpha.-hydroxyaldehyde.

IT 128387-05-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (enantiopure aminotriol from isoascorbic acid synthesis of threosphingosine)

RN 128387-05-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-,
[R-[R*,R*-(E)]]- (9CI) (CA INDEX NAME)
Searched by Barb O'Bryen & Toby Port

Absolute stereochemistry. Double bond geometry as shown.

L32 ANSWER 12 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1996:190105 CAPLUS

DOCUMENT NUMBER: 124:342900

TITLE: Diastereoselective synthesis of triacetyl-L-erythro-

C18-sphingosine

AUTHOR(S): Miyata, Okiko; Yamaguchi, Sayaka; Ninomiya, Ichiya;

Naito, Takeaki; Okamura, Kimio

CORPORATE SOURCE: Kobe Pharmaceutical Univ., Higashinada, 658, Japan

SOURCE: Chem. Pharm. Bull. (1996), 44(3), 636-8

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:342900

AB A new stereoselective synthetic route to triacetyl-L-erythro-C18-

sphingosine has been developed by the combination of diastereoselective

addn. of thiophenol to chiral olefins and subsequent intramol.

substitution of the corresponding sulfonium group.

IT 2482-37-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(stereoselective prepn. of triacetyl-L-erythro-C18-sphingosine)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-

heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 13 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1996:113258 CAPLUS

DOCUMENT NUMBER: 124:176808

TITLE: Preparation of sphingosine derivatives

INVENTOR(S): Murakami, Teiichi; Namikawa, Hiroyuki; Hado, Masakatsu

PATENT ASSIGNEE(S): Kogyo Gijutsuin, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent

LANGUAGE: Patent Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE ______ ____ _____ _____ JP 07258178 A2 19951009 JP 1994-74085 19940318 JP 2560250 B2 19961204 OTHER SOURCE(S): CASREACT 124:176808; MARPAT 124:176808

$$N = \begin{pmatrix} Ph \\ N = \begin{pmatrix} O \\ O \end{pmatrix} \end{pmatrix}$$
OH III

The title compds. I [R1 - R3 = H] are prepd. in a multistep process. Thus, acetalization of N-benzoyl-D-glucosamine, followed by redn., sulfonylation, formation of oxazoline moiety, deacetalization, gave oxazoline derivs. II [R = alkyl]. II was converted in several steps to oxazoline deriv. III. III was treated with HCl in THF at room temp. for 20 h. NaOH, EtOH, and water were added to the reaction mixt. which was then stirred at 95.degree. for 16 h to give, after workup, I [R1 = R2 = R3 = H].

IT 2482-37-3P

GΙ

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(prepn. of sphingosine derivs.)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 14 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1995:958040 CAPLUS

DOCUMENT NUMBER: 124:768

TITLE: Pharmaceutically active sphingolipid compounds,

liposomes containing them, and methods of use,

especially for treatment of cancer

INVENTOR(S): Pei, Yong-Wei; Mayhew, Eric; Ahmad, Imran; Janoff,

Andrew S.

PATENT ASSIGNEE(S): Liposome Co., Inc., USA

Liposome Co., Inc., USA Searched by Barb O'Bryen & Toby Port SOURCE:

PCT Int. Appl., 64 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PAT	ENT NO.		KIND	DATE		APPLICATION NO.	DATE	
WO	9521175 W: AU,					WO 1995-US1490	19950202	
	RW: AT,	BE, C	H, DE,	DK, ES,		GB, GR, IE, IT, LU,		SE
CA .	2182485		AA	19950810		CA 1995-2182485	19950202	
AU	9518712		A1	19950821		AU 1995-18712	19950202	
AU	691886		В2	19980528				
EP	742789		A1	19961120		EP 1995-910923	19950202	
	R: AT,	BE, C	H, DE,	DK, ES,	FR,	GB, GR, IE, IT, LI,	LU, MC, NL,	PT, SE
JP	09508900		Т2	19970909		JP 1995-520799	19950202	,
EP	1008342		A2	20000614		EP 2000-102434	19950202	
	R: AT,	BE, C	H, DE,	DK, ES,	FR,	GB, GR, IT, LI, LU,	NL, SE, MC,	PT, IE
FΙ	9603045		A	19960801		FI 1996-3045	19960801	•
МО	9603224		A	19960927		NO 1996-3224	19960801	
PRIORITY	APPLN.	INFO.:				US 1994-190295	19940202	
				-		EP 1995-910923	19950202	
						WO 1995-US1490	19950202	

OTHER SOURCE(S): MARPAT 124:768

Compds. R1Y1CHZ1CH(NY2Y3)CH2Z2 [R1 = straight-chain C8-19 alkyl, alkenyl or alkynyl; Y1 = CH=CH, C||C, CH(OH)CH(OH); Z1 = OH, conversion-inhibiting group; Z2 = conversion-inhibiting group; Y2 = H, Ph, (C1-6 alkyl)-substituted Ph, C1-6 alkyl; Y3 = H, C(0)R2, -S(0)2R2; R2 = straight-chain C1-23 alkyl, alkenyl or alkynyl; when Z2 = amino, R2 = C1-9 or C19-23 aliph. chain] are disclosed, as are liposomes contg. such compds. Methods for treating cancer using the compds. and liposomes of the invention are also disclosed. The effect of e.g. various liposomal ceramide/sphingomyelin formulations on the growth of e.g. HL-60 cells was detd.

170925-95-8 170925-96-9 170925-97-0 IT 170925-98-1 170925-99-2 170926-01-9 170926-08-6 170926-09-7 170926-10-0

> RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(sphingolipid compds., liposomes contg. them, and methods of use, esp. for cancer therapy)

RN170925-95-8 CAPLUS

CN Hexanamide, N-[1-[(acetyloxy)methyl]-2-hydroxy-3-heptadecenyl]-, $[R-[R^*,S^*-(E)]]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN . 170925-96-9 CAPLUS

CN Hexanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

$$ACO$$
 R
 E
 $(CH_2)_{12}$
 Me
 OAC
 $(CH_2)_{12}$
 Me

RN 170925-97-0 CAPLUS

CN Butanoic acid, 3-hydroxy-2-[(1-oxohexyl)amino]-4-octadecenyl ester, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 170925-98-1 CAPLUS

CN Propanoic acid, 2-methyl-, 3-hydroxy-2-[(1-oxohexyl)amino]-4-octadecenyl ester, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Me (CH₂)
$$\frac{1}{4}$$
 E R S O Pr-i

RN 170925-99-2 CAPLUS

CN Hexanamide, N-[1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 170926-01-9 CAPLUS

CN Hexanamide, N-[2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-heptadecenyl]-, [R-[R*,S*-(E)]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

Me (CH₂)₁₂
$$\stackrel{E}{\underset{\text{T-Bu}}{=}}$$
 $\stackrel{O}{\underset{\text{Ne}}{=}}$ $\stackrel{O}{\underset{\text{Me}}{=}}$ $\stackrel{Me}{\underset{\text{Me}}{=}}$ $\stackrel{CH_2)_{12}}{\underset{\text{Me}}{=}}$ $\stackrel{E}{\underset{\text{Me}}{=}}$ $\stackrel{O}{\underset{\text{Me}}{=}}$ $\stackrel{Me}{\underset{\text{Me}}{=}}$ $\stackrel{Me}{\underset{\text{Me}}{=}}$

RN 170926-08-6 CAPLUS

CN Acetamide, N-[1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 170926-09-7 CAPLUS

CN Acetamide, N-[1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 170926-10-0 CAPLUS

CN Hexanamide, N-[2-(acetyloxy)-1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-3-heptadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

L32 ANSWER 15 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1995:819842 CAPLUS

DOCUMENT NUMBER:

124:30186

TITLE:

Diastereo- and enantioselective synthesis of L-threo-

and D-erythro-sphingosine

AUTHOR(S):

Enders, Dieter; Whitehouse, Darren L.; Runsink, Jan

CORPORATE SOURCE:

Inst. Organische Chemie, Technischen Hochschule,

Aachen, D-52074, Germany

SOURCE:

Chem. -- Eur. J. (1995), 1(6), 382-8

Published in: Angew. Chem., Int. Ed. Engl., 34, 17

CODEN: CEUJED; ISSN: 0947-6539

DOCUMENT TYPE:

LANGUAGE:

Journal

English

GΙ

$$NH_2$$
 $C_{13}H_{27}$ OH I Me Me II

- AB Asym. synthesis of L-threo-sphingosine and its D-erythro isomer I via aldol reaction of the SAMP hydrazone (S)-II with racemic .alpha.-phenylselenylpentadecanal Me(CH2)12(SePh)CHO is reported.
- TT 78779-96-1P 116612-39-6P

 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

 Searched by Barb O'Bryen & Toby Port

(diastereo- and enantioselective synthesis of L-threo- and D-erythro-sphingosine)

78779-96-1 CAPLUS RN

Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-CN heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 116612-39-6 CAPLUS

CN Acetamide, N-[1-[(acetyloxy)methyl]-2-hydroxy-3-heptadecenyl]-, $[S-[R^*,R^*-(E)]]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

IT 2482-37-3P

> RL: SPN (Synthetic preparation); PREP (Preparation) (diastereo- and enantioselective synthesis of L-threo- and D-erythro-sphingosine)

2482-37-3 CAPLUS RN

Acetamide, N-[(1S, 2R, 3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-CN heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 16 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER:

1995:520214 CAPLUS

DOCUMENT NUMBER:

123:83890

TITLE:

Sphingolipid bases. A revisitation of the O-methyl

derivatives of sphingosine. Isolation and

characterization of diacetate derivatives, with

revised 13C nuclear magnetic resonance assignments for

D-erythro-sphingosine

AUTHOR (S):

Kisic, Alemka; Tsuda, Mitsuhiro; Kulmacz, Richard J.;

Wilson, William K.: Schroepfer, George J., Jr. Searched by Barb O'Bryen & Toby Port

CORPORATE SOURCE:

Dep. Biochemistry, Rice Univ., Houston, TX, 77251, USA

J. Lipid Res. (1995), 36(4), 787-803

CODEN: JLPRAW; ISSN: 0022-2275

DOCUMENT TYPE:

Journal

LANGUAGE:

SOURCE:

English

GΙ

AB Isolation by medium pressure liq. chromatog. and mol. structure of D-erythro-sphingosine diacetates, e.g. I (R = H, Ac), are reported. Structures were detd. by phys., chromatog., and spectral properties. The 5-O-Me ethers, which were the predominant byproducts of sphingolipid hydrolysis, were easily distinguished from the 3-O-Me ethers by chromatog., and all four isomers could be differentiated by 1H and 13C NMR (NMR) spectroscopy. Resoln. enhancement of the 126-MHz 13C NMR spectra of the O-Me ethers and D-erythro-C18-sphingosine I (R = H) afforded distinct signals for nearly all carbon atoms. 13C NMR assignments of carbons 7-15 were made from their lanthanide-induced shifts, and revised assignments for olefinic carbons at I (R = H) were established based upon 1H-13C shift correlation expts.

IT 2482-37-3 78779-96-1

RL: PRP (Properties)

(isolation and mol. structure characterization of D-erythro-sphingosine diacetates)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

L32 ANSWER 17 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER:

1995:229666 CAPLUS

DOCUMENT NUMBER:

122:133593

TITLE:

Chemoenzymic Synthesis of D-erythro- and

L-threo-C18-Sphingosines

AUTHOR(S):

Hudlicky, Tomas; Nugent, Thomas; Griffith, William

Department of Chemistry, Virginia Polytechnic

Institute and State University, Blacksburg, VA, 24061,

SOURCE:

J. Org. Chem. (1994), 59(26), 7944-6

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE:

CORPORATE SOURCE:

Journal

LANGUAGE:

English

GI

$$R$$
 R^1 R^1

Two sphingosine stereoisomers, the natural isomer I (R = H, R1 = OH) and AΒ the L-threo isomer I (R = OH, R1 = H), were prepd. from azido alcs. II via biol. oxidn. of chlorobenzene with toluene dioxygenase from the whole cells of Pseudomonas putida 39D.

78779-96-1P IT

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of sphingosine stereoisomers via stereoselective toluene

dioxygenase oxidn. of chlorobenzene)

78779-96-1 CAPLUS RN

Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-CN heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

CAPLUS COPYRIGHT 2000 ACS ANSWER 18 OF 72

ACCESSION NUMBER:

1994:533751 CAPLUS

DOCUMENT NUMBER:

121:133751

TITLE:

Regio- and stereocontrolled synthesis of

D-erythro-sphingosine and phytosphingosine from

D-glucosamine

AUTHOR (S):

Murakami, Teiichi; Minamikawa, Hiroyuki; Hato,

CORPORATE SOURCE:

Natl. Inst. Mater. Chem. Res., Tsukuba, 305, Japan

SOURCE:

Tetrahedron Lett. (1994), 35(5), 745-8

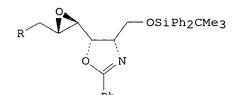
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE:

Journal

LANGUAGE:

English



AB D-Erythro-sphingosine (I) and phytosphingosine (II) have been efficiently synthesized from D-glucosamine by utilizing its whole carbon skeleton and functional groups. In this synthetic route, regioselective alkylation of the epoxy tosylate III [R = 4-MeC6H4SO3] was achieved with a copper(I)-catalyzed Grignard reagent to give the key intermediate III [R = (CH2)11Me], which was converted to both I and II via regioselective formation of the iodohydrin IV.

IT 2482-37-3P

III

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 19 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER:

1994:436061 CAPLUS

DOCUMENT NUMBER:

121:36061

TITLE:

A Four-Step Diastereoselective Synthesis of

D-erythro-Sphingosine by an Enantioselective Aldol Reaction Using a Titanium Enolate Derived from a

Chiral Iminoglycinate

AUTHOR(S):

SOURCE:

Solladie-Cavallo, Arlette; Koessler, Jean L.

CORPORATE SOURCE: Laboratoire de Stereochimie Organometallique, E.H.I.C.S., Strasbourg, 67008, Fr.

J. Org. Chem. (1994), 59(11), 3240-2

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 121:36061

GΙ

AB A 4-step synthesis of D-erythro-sphingosine I, with recovery of the chiral auxiliary, is described. The detg. step is a diastereo- and enantioselective aldol reaction using a directly-generated titanium enolate.

IT 2482-37-3P

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 20 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER:

1994:226633 CAPLUS

DOCUMENT NUMBER:

120:226633

TITLE:

Three glycosphingolipids having the phosphocholine

group from the crude drug "Jiryu" (the earthworm,

Pheretima asiatica)

AUTHOR(S):

Noda, Naoki; Tanaka, Ryuichiro; Miyahara, Kazumoto;

Kawasaki, Toshio

CORPORATE SOURCE:

Fac. Pharm. Sci., Setsunan Univ., Hirakata, 573-01,

Japan

SOURCE:

Chem. Pharm. Bull. (1993), 41(10), 1733-7

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GΙ

AB Three glycosphingolipids were isolated in the pure state from the crude drug, "Jiryu" (the earthworm, Pheretima asiatica). Their structures were detd. as I-III. They are zwitterionic glycosphingolipids having a phosphocholine group attached to the sugar moiety, resembling those obtained from two kinds of marine annelid, and one has a branched long-chain base.

IT 2482-37-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 21 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1993:427905 CAPLUS

DOCUMENT NUMBER: 119:27905

TITLE: Stereoselective synthesis of D-(+)-erythro- and

L-(-)-threo-Sphingosines from carbohydrates

AUTHOR(S): Yadav, J. S.; Vidyanand, D.; Rajagopal, D.

CORPORATE SOURCE: Indian Inst. Chem. Technol., Hyderabad, 500007, India

SOURCE: Tetrahedron Lett. (1993), 34(7), 1191-4

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: English

GΙ

AB Stereocontrolled syntheses of D-(+)-erythro and L-(-)-threo-sphingosines I (R = H, R1 = H0; R = H0, R1 = H resp) are described starting from D-xylose and D-arabinose resp. through acetvlenic intermediates II (same R, R1), Searched by Barb O'Bryen & Toby Port

obtained by base induced double elimination of the .beta.-alkoxy chlorides, e.g. III.

IT 78779-96-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAMÉ)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

L32 ANSWER 22 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1993:45757 CAPLUS

DOCUMENT NUMBER: 118:45757

TITLE: Amino alcohol derivatives as membrane penetration

enhancers

INVENTOR(S): Rajadhyaksha, Vithal J.

PATENT ASSIGNEE(S): USA

SOURCE: PCT Int. Appl., 43 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO. WO 9216236			KIND DA		DATE	DATE			APPLICATION NO.				DATE		
				Α.	1	1992	1001		WO 1992-US2219			9	19920319			
		W:	AU,	CA,	JP											
		RW:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB, GR,	IT,	LU,	MC,	NL,	SE	
	CA	2106	483		A	A.	1992	0920		CA 19	992-2	10648	83	19920	319	
	ΑU	9217	451		A	1	1992	1021		AU 19	992-1	7451		19920	319	
	ΑU	6641	78		B	2	1995	1109								
	EΡ	5766	05		A	1	1994	0105		EP 19	992-9	10289	9	19920	319	
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB, GR,	IT,	LI,	LU,	MC,	NL,	SE
	JΡ	0650	9559		\mathbf{T}^{2}	2	1994	1027		JP 19	992-5	0996	4	19920	319	
	US	5482	965		Α		1996	0109		US 19	993-1	15772	2	1993	0903	
PRIO	RIT:	APP	LN.	INFO	. :					US 19	91-6	72020	0	1991	319	
										WO 19	992-U	5221	9	19920	0319	

OTHER SOURCE(S): MARPAT 118:45757

GΙ

AB Amino alcs., including dioxane derivs., are prepd. as penetration enhancers for topical pharmaceuticals. I was prepd. from 2-ethylhexanal and 5-nitro-1,3-dioxane and redn. of the product. An analgesic gel was prepd. contg. Carbopol 941 1.5, diclofenac Na 1, 2-propanol 35, diisopropanolamine 1.8, diisopropyl adipate 5, I 2, and water 53.7%.

IT 96579-26-9 145277-15-2

RL: BIOL (Biological study)

(penetration enhancer, for topical pharmaceuticals)

RN 96579-26-9 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

RN 145277-15-2 CAPLUS

CN Octadecanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-(9CI) (CA INDEX NAME)

L32 ANSWER 23 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER:

1992:571846 CAPLUS

DOCUMENT NUMBER:

117:171846

TITLE:

Sphingolipids and glycerolipids. II. Syntheses of two pairs of enantiomeric C18-sphingosines and a palmitoyl analog of Gaucher spleen glucocerebroside Shibuya, Hirotaka; Kawashima, Keiko; Narita, Norihiko;

AUTHOR(S):

Ikeda, Masahiko; Kitagawa, Isao

CORPORATE SOURCE:

Fac. Pharm. Sci., Osaka Univ., Suita, 565, Japan

SOURCE:

Chem. Pharm. Bull. (1992), 40(5), 1154-65

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI

AB Sixteen chiral C4 epoxides I (R = 4-MeOC6H4CPh2. PhCH2. MeOCH2, Searched by Barb O'Bryen & Toby Port

Me3CSiMe2), which are synthons for complex lipids, have been prepd. from (2Z)-2-butene-1,4-diol by employing a Sharpless asym. epoxidn. By using I as starting compds., two pairs of enantiomeric C18 sphingosines (E)-HOCH2CH(NH2)CH(OH)CH:CH(CH2)12Me (II) have been synthesized via a regioselective ring-opening of the epoxide ring with azide anion followed by redn. of the azide group to an amino group and a Wittig reaction. Furthermore, D-erythro-II has been converted to the palmitoyl analog III of Gaucher spleen glucocerebroside through a reaction pathway including successive condensations with palmitic acid and D-glucose.

IT 143517-08-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and benzoylation of)

RN 143517-08-2 CAPLUS

CN Hexadecanamide, N-[(1S,2R,3E)-1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]me thyl]-2-hydroxy-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

IT 2482-37-3P 128387-02-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and deblocking of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 128387-02-0 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

IT 78779-96-1P 128387-01-9P 128387-05-3P 143615-68-3P

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 128387-01-9 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R-[R*,S*-(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 128387-05-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R-[R*,R*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 143615-68-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,S*-(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

L32 ANSWER 24 OF 72 CAPLUS COPYRIGHT 2000 ACS

1992:571057 CAPLUS ACCESSION NUMBER:

117:171057 DOCUMENT NUMBER:

Aluminoxy acetals from .alpha.-amino esters: TITLE:

> chirality transfer via sequential addition of hydride and C-nucleophiles. 2-Amino alcohols and sphingosines

Polt, Robin; Peterson, Matt A.; DeYoung, Lynn AUTHOR (S):

CORPORATE SOURCE: Dep. Chem., Univ. Arizona, Tucson, AZ, 85721, USA

SOURCE: J. Org. Chem. (1992), 57(20), 5469-80

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:171057

The reaction of .alpha.-imino esters with aluminum hydrides to produce AB acetal-like intermediates and subsequent reaction with carbon nucleophiles has been studied. Treatment of optically pure imine-protected amino esters with i-Bu2AlH or i-Bu2AlH.cntdot.i-Bu3Al, followed by RMgX or RLi provided threo-2-amino alcs. in high yield (73-85%) and excellent syn stereoselectivity (8:1 to >20:1, threo or threo-like product preferred). Use of nonpolar solvents (CH2Cl2-hexane) provided the highest stereoselectivities. Use of the less-reactive i-Bu2AlH.cntdot.i-Bu3Al complex lowered the amt. of undesired primary alc. products obsd. Thermally labile aluminoxy acetal intermediates were obsd. by 1H NMR and were trapped with N-(trimethylsilyl)imidazole to produce relatively stable monosilyl acetals (mixed acetals). Alanine-derived Schiff bases (S)-Ph2C:NCHMeCO2R (I; R = Me, Et, CH2Ph, CHPh2, CMe3) showed a correlation between the steric bulk of the ester and threo selectivity. The presence of THF reduced this correlation, suggesting the C-nucleophile addn. involves a Lewis acid-assisted SN2-like displacement of the aluminoxy acetal or displacement of a tight-ion pair. In addn. to the synthesis of optically pure arylethanolamines II (R1 = H, Me, CH2Ph, CH2OSiMe2CMe3) from representative amino acids, threo-sphingosines III (R2 = OSiMe2CMe3, n = 3, 4, 7, 12) were synthesized from L-serine-derived Schiff base (S)-Ph2C:NCH(CH2OSiMe2CMe3)CO2Me, and 1-deoxy-threosphingosines III (R2 = H, n = same) were synthesized from I (R = Me) in a similar fashion. Exptl. details are provided. IT

78779-96-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

L32 ANSWER 25 OF 72 CAPLUS COPYRIGHT 2000 ACS

1992:59850 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 116:59850

The synthesis of glycosphingolipids: I. The TITLE:

synthesis of lactosylceramide and lactosylsphingenine

and a short synthesis of triacetyl-D-erythro-

sphingosine. II. The synthesis of the Lex family of

glycosphingolipids

Caulfield, Thomas Joseph AUTHOR(S):

Univ. Pennsylvania, Philadelphia, PA, USA CORPORATE SOURCE:

(1991) 358 pp. Avail.: Univ. Microfilms Int., Order SOURCE:

No. DA9125609

From: Diss. Abstr. Int. B 1991, 52(3), 1432

DOCUMENT TYPE: Dissertation

LANGUAGE: English

Unavailable AB 2482-37-3P IΤ

RN

AUTHOR (S):

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of) 2482-37-3 CAPLUS

Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-CN

(CA INDEX NAME) heptadecenyl] - (9CI)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

CAPLUS COPYRIGHT 2000 ACS L32 ANSWER 26 OF 72

ACCESSION NUMBER: 1992:41172 CAPLUS

DOCUMENT NUMBER: 116:41172

Enantiospecific syntheses of sphingosine and ceramide TITLE:

stereoisomers with 3S configuration from D-glucose Fujita, Shuji; Sugimoto, Mamoru; Tomita, Kenkichi;

Nakahara, Yoshiaki; Ogawa, Tomoya CORPORATE SOURCE:

MECT Corp., Saitama, 359, Japan SOURCE:

Agric. Biol. Chem. (1991), 55(10), 2561-9

CODEN: ABCHA6; ISSN: 0002-1369

DOCUMENT TYPE: Journal Searched by Barb O'Bryen & Toby Port LANGUAGE:

English

GΙ

AB Starting from D-glucose, 2-amino-4-octadecene-1,3-diols I (R = H, R1 = NH2; R = NH2, R1 = H) and 4 stereoisomers of tetracosanoylsphingenine II were prepd.

IT 121468-17-5P 121468-18-6P

RN 121468-17-5 CAPLUS

CN Tetracosanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,R*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 121468-18-6 CAPLUS

CN Tetracosanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,R*-(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

L32 ANSWER 27 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1991:680423 CAPLUS

DOCUMENT NUMBER: 115:280423

TITLE: A convenient stereoselective synthesis of

D-erythro-C18-sphingosine from galactal

AUTHOR(S): Hirata, Norihiko; Yamagiwa, Yoshiro; Kamikawa, Tadao

CORPORATE SOURCE: Fac. Sci. Technol., Kinki Univ., Higashi-Osaka, 577,

Japan

SOURCE: J. Chem. Soc. Perkin Trans. 1 (1991). (9), 2279-80

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: LANGUAGE: Journal English

OTHER SOURCE(S):

CASREACT 115:280423

GΙ

$$C_{13}H_{27}$$

AB The highly efficient stereoselective synthesis of title sphingosine I from 3,4,6-tribenzyloxygalactal in 9 steps and 26% overall yield, via 4,6-tribenzyloxy-5-hydroxyhexenal, is described.

IT 2482-37-3P

AUTHOR (S):

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 28 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1991:626541 CAPLUS

DOCUMENT NUMBER: 115:226541

TITLE: Interaction of cholesterol with synthetic

sphingomyelin derivatives in mixed monolayers Gronberg, Lotte; Ruan, Zhongshi; Bittman, Robert;

Slotte, J. Peter

CORPORATE SOURCE: Dep. Biochem. Pharm., Abo Akad. Univ., Turku,

SF-20500, Finland

SOURCE: Biochemistry (1991), 30(44), 10746-54

CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal LANGUAGE: English

AB To study the structural requirements of the mol. interactions between cholesterol and sphingomyelins in model membranes, sphingomyelin derivs. were synthesized in which (a) the 3-hydroxy group was replaced with a hydrogen atom or with a methoxy, ethoxy, or tetrahydropyranyloxy group, (b) the N-acyl chain length was varied, and (c) the N-acyl chain length contained an .alpha.-hydroxy group. The chem. syntheses of these derivs. from DL-erythro-sphingosine are reported. The properties of these sphingomyelin derivs. were examd. in monolayer membranes at the air/water interface. The mean mol. area of the pure N-stearoylsphingomyelin derivs. was detd., and the effects of cholesterol on the condensation of sphingomyelin packing in the monolayer were recorded. It was obsd. that replacement of the 3-hydroxy group of sphingomyelin with a hydrogen atom Searched by Barb O'Bryen & Toby Port

or its substitution with a methoxy or ethoxy group did not affect the ability of cholesterol to condense the mol. packing in monolayers. when a bulky tetrahydropyranyloxy group was introduced at the 3-hydroxy position of egg sphingomyelin, cholesterol was still able to condense the mol. packing of this deriv. The condensing effect of cholesterol on derivs. of N-stearoylsphingomeylins was significantly larger than the comparable effect obsd. with 1,2-distearoyl-sn-glycero-3-phosphocholine or 1,2-dipalmitoyl-sn-glycero-3-phosphocholine. Results with 3-hydroxysphingomyelins having differing N-acyl chain lengths (i.e., N-stearoyl, N-myristoyl, and N-lauroyl), and with 3-hydroxy-N-(.alpha.hydroxypalmitoyl)sphingomyelin also indicated that cholesterol was able to induce condensation of the mol. packing. Another measure of the mol. packing in monolayers is the cholesterol oxidase susceptibility of cholesterol embedded in sphingomyelin-contg. monolayers. The rate of enzyme-catalyzed cholesterol oxidn. in monolayers contg. 3-hydroxy-substituted N-stearoylsphingomyelins was about 30% lower than the comparable maximal rate measured in a monolayer of dipalmitoylphosphatidylcholine at the same surface pressure. Substitution of a hydroxy group at the .alpha. position of the amide chain of sphingomyelin did not perturb the projection of the sterol's 3.beta.-hydroxy group toward the lipid/water interface. Cholesterol was, however, oxidized about 50% faster in monolayers contg. 3-hydroxysphingomyelins with shorter acyl chains (i.e., N-lauroyl and N-myristoyl) than with a N-stearoyl chain, the rate being similar to that obsd. in a dipalmitoylphosphatidylcholine/cholesterol mixed monolayer. It is concluded that the 3-hydroxy group of sphingomyelin is not required for the efficient interaction between cholesterol and sphingomyelin in monolayer membranes. Furthermore, shortening the N-acyl group of sphingomyelin by 4 to 6 methylene groups had only a marginal effect on this interaction in monolayers.

IT 136794-89-3P 136794-91-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and conversion to tetrahydropyranyl deriv.)

RN 136794-89-3 CAPLUS

CN Tetradecanamide, N-[1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]-, [R*,S*-(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

RN 136794-91-7 CAPLUS

CN Dodecanamide, N-[1-[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]-, [R*,S*-(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

L32 ANSWER 29 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1991:470908 CAPLUS

DOCUMENT NUMBER: 115:70908

TITLE: Total synthesis of chiral 2-amino-1,3-diols

INVENTOR(S): Illig, Carl R.; Weis, Alexander L.

PATENT ASSIGNEE(S): Eastman Kodak Co., USA

SOURCE: U.S., 9 pp. CODEN: USXXAM

DOCUMENT TYPE: Patent English LANGUAGE:

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	<u> </u>			
US 5012000	Α	19910430	US 1989-428799	19891030

CASREACT 115:70908 OTHER SOURCE(S):

D-erythro-Sphingosine was prepd. in a 4 step synthesis from AΒ (S)-3-(chloroacetyl)-4-benzyl-2-oxazolidinone by sequential aldol condensation with trans-2-hexadecenal, azide substitution reaction, NaBH4 redn. and azide redn. with HS(CH2)3SH and Et3N.

IT 2482-37-3P

> RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 2482-37-3 CAPLUS

Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-CN heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 30 OF 72 CAPLUS COPYRIGHT 2000 ACS

1991:466885 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 115:66885

TITLE: Interaction of cholesterol with sphingomyelin in

bilayer membranes: evidence that the hydroxy group of

sphingomyelin does not modulate the rate of

cholesterol exchange between vesicles

Kan. Chu Cheng; Ruan. Zhong Shi; Bittman, Robert Searched by Barb O'Bryen & Toby Port AUTHOR (S):

CORPORATE SOURCE:

Queens Coll., City Univ. New York, Flushing, NY,

11367, USA

SOURCE:

Biochemistry (1991), 30(31), 7759-66

CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE:

Journal

English LANGUAGE: AB

Cholesterol undergoes exchange between membranes contg. sphingomyelin at a much slower rate than between membranes lacking sphingomyelin. investigate the role of the hydroxy group at the 3-position of sphingomyelin in the interaction between sphingomyelin and cholesterol, the rates of [4-14C]cholesterol exchange were measured between unilamellar vesicles prepd. with N-stearoylsphingomyelin or with synthetic analogs in which the hydroxy group is replaced with an O-alkyl group or with hydrogen. Vesicles prepd. from 3-deoxy- and 3-0-methyl-Nstearoylsphingomyelin had the same rate of [14C]cholesterol desorption. The half-times for exchange from vesicles prepd. with 3-0-methyl- and 3-deoxy-N-stearoylsphingomyelins and 10 mol % of cholesterol were only slightly faster (a factor of only 1.5) than that found from vesicles prepd. from N-stearoylsphingomyelin and 10 mol % cholesterol. The rate of cholesterol desorption from vesicles could be accelerated by prepg. vesicles from bulky 3-O-alkyl analogs of sphingomyelin. Vesicles contg. 3-O-ethyl-N-stearoylsphingomyelin and 3-O-tetrahydropyranyl egg sphingomyelin gave rate enhancements of .apprx.14 and 35, compared with the rates obsd. in vesicles made from N-stearoyl- and egg sphingomyelin, resp. These data indicate that insertion of sterically bulky groups at the 3-position of sphingomyelin (such as ethoxy and tetrahydropyranyloxy) in place of hydroxy interferes markedly with the mol. packing of cholesterol and sphingomyelin in bilayer membranes; however, the hydroxy group of sphingomyelin is not crit. for the strong interaction of cholesterol with sphingomyelin. These results suggest that van der Waals interactions are more important than hydrogen-bonding interactions involving the hydroxy group in contributing to tight lateral packing of cholesterol with sphingomyelin.

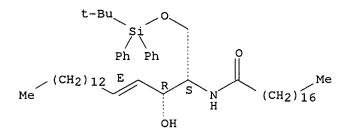
IT 134654-02-7P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and reaction with Me iodide)

134654-02-7 CAPLUS RN

Octadecanamide, N-[1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-CN hydroxy-3-heptadecenyl]-, [R*,S*-(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry. Double bond geometry as shown.



L32 ANSWER 31 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER:

1991:429780 CAPLUS

DOCUMENT NUMBER:

115:29780

TITLE:

Synthesis of sphingosine relatives. X. Synthesis of (2S, 3R, 4E)-1-0-(.beta.-D-glucopyranosyl)-N-[30'-(linoleoyloxy) triacontanoyl]-4-icosasphingenine, a new esterified cerebroside isolated from human and pig Searched by Barb O'Bryen & Toby Port

epidermis

AUTHOR(S):

Mori, Kenji; Matsuda, Hiroyuki

CORPORATE SOURCE:

Dep. Agric. Chem., Univ. Tokyo, Tokyo, 113, Japan

Ι

Liebigs Ann. Chem. (1991), (6), 529-35

CODEN: LACHDL; ISSN: 0170-2041

DOCUMENT TYPE: LANGUAGE: Journal English

GI

SOURCE:

HO HO (CH₂)₁₄Me (CH₂)₄Me (CH₂)₄Me (CH₂)₄Me

AB Glucopyranosylicosasphingenine I was synthesized from D-glucose, L-serine, 15-pentadecanolide, and linoleic acid. The high-field 1H NMR spectrum of I was identical with that of the esterified cerebroside isolated from human and pig epidermis.

IT 25494-35-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 25494-35-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

L32 ANSWER 32 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER:

1991:229262 CAPLUS

DOCUMENT NUMBER:

114:229262

TITLE:

Asymmetric synthesis via heterocyclic intermediates. 43. Asymmetric synthesis of D-erythro-sphingosine Groth, Ulrich; Schoellkopf, Ulrich; Tiller, Thomas

AUTHOR(S):
CORPORATE SOURCE:

Inst. Org. Chem., Univ. Goettingen, Goettingen,

D-3400, Fed. Rep. Ger.

SOURCE:

Tetrahedron (1991), 47(16-17), 2835-42

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 114:229262

GΙ

AB Title compd. I is a building block of cerebrosides and glycosphingolipids and was synthesized in 5 steps via an asym. aldol addn. of the inhibited bislactim ether of II to (2E)-hexadecenal in an overall yield of 21 %.

IT 2482-37-3P

> RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1s, 2r, 3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 33 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER:

1991:207692 CAPLUS

DOCUMENT NUMBER:

114:207692

TITLE:

Preparation of unnatural sialosylceramides

INVENTOR(S):

Fujita, Hideji; Sugimoto, Mamoru; Ito, Masayoshi;

Ogawa, Tomoya

PATENT ASSIGNEE(S):

Mekuto K. K., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 16 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02202895	A2	19900810	JP 1989-23290	19890201
OTHER SOURCE(S):	MA	RPAT 114:207692		

GI

$$\begin{array}{c} \text{OR}^1 \\ \text{R}^{10} \\ \text{AcNH} \\ \text{R}^{10} \\ \text{I} \end{array} \begin{array}{c} \text{OR}^4 \\ \text{OR}^4 \\ \text{C}_{13}\text{H}_{27} \\ \text{NHCOC}_{23}\text{H}_{47} \end{array}$$

AB The title compds. [I; R1 = acyl, H; R2, R3 = Q, CO2R5; R4 = H, Bz; provided that R2 and R3 may not be simultaneously the same; R5 = alkyl, alk. metal], useful for studying animal cell proliferation (no data), were prepd. via condensation of the appropriate sugar acid derivs. with ceramides HQ. A mixt. of I [R1 = Ac, R2 = C1, R3 = CO2Me], HQ [R4 = Bz] (prepn. given), Hg(CN)2, HgBr2, mol. sieve 4A, and CHCl3 was heated in an oil bath at 50.degree. for 2 h gave I [R1 = Ac, R2 = CO2Me, R3 = Q, R4 = Bz].

IT 121468-17-5P 121468-18-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as intermediate for unnatural sialosylceramides)

RN 121468-17-5 CAPLUS

CN Tetracosanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,R*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 121468-18-6 CAPLUS

CN Tetracosanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,R*-(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

Me (CH₂)₁₂
$$\overline{z}$$
 \overline{s} \overline{N} \overline{N} (CH₂)₂₂ \overline{N} \overline{N}

L32 ANSWER 34 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1991:161128 CAPLUS

DOCUMENT NUMBER: 114:161128

TITLE: Cerebrosides of from brain. Structure of the ceramide Searched by Barb O'Bryen & Toby Port

part of the cerebrosides

AUTHOR(S): Munesada, Kiyotaka; Yuasa, Masatoshi; Suga, Takayuki CORPORATE SOURCE: Fac. Sci., Hiroshima Univ., Hiroshima, 730, Japan J. Chem. Soc., Perkin Trans. 1 (1991), (1), 189-94

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal LANGUAGE: English

AB Twelve cerebrosides were isolated from the brain tissues of the bullfrog (Bana catesbeiana) and were characterized as 1-o-.beta.-D-galactopyranosyl ceramides. On the basis of chem. and spectral evidence, the ceramide parts of six of them were found to be composed of a sphingosine as a long-chain base and six fatty acids consisting of C18:0, C22:1, and C24:1 acids and their 2-hydroxy derivs. The ceramide parts of the others were found to be composed of a dihydroxsphingosine and the six fatty acids. The configurations at C-2 and C-3 of the two long-chain bases were detd. to be S and R, resp. A different distribution of the cerebrosides was seen among the hemisphere, diencephalon and mixed tissue from the optic lobe, cerebellum and medulla oblongata of the brain.

IT 2482-37-3P

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 35 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1991:120954 CAPLUS

DOCUMENT NUMBER: 114:120954

TITLE: Asymmetric aldol reaction catalyzed by chiral

complexes

AUTHOR(S): Hayashi, Tamio; Ito, Yoshihiko

CORPORATE SOURCE: Grad. Sch. Pharm. Sci., Hokkaido Univ., Sapporo, 060,

Japan

SOURCE: Yukagaku (1990), 39(10), 846-51

CODEN: YKGKAM; ISSN: 0513-398X

DOCUMENT TYPE: Journal LANGUAGE: Japanese

OTHER SOURCE(S): CASREACT 114:120954

AB Asym. aldol reactions of .alpha.-isocyano carboxylates with aldehydes were catalyzed by gold(I) complexes with a chiral ferrocenylphosphine ligand contg. a [(dialkylamino)ethyl]amino group on the ferrocene side chain. Optically active (up to 98% ee) 5-alkyl-trans-4-(methoxycarbonyl)-2-oxazolines were obtained with high enantio- and diastereoselectivity in quant. yield. The optically active oxazolines were readily converted to .beta.-hydroxy-.alpha.-amino acids and their derivs.

IT 78779-96-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetvloxv)-1-[(acetvloxv)methvl]-3-Searched by Barb O'Bryen & Toby Port heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

L32 ANSWER 36 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1990:531846 CAPLUS

DOCUMENT NUMBER: 113:131846

TITLE: Synthesis of two pairs of enantiomeric

C18-sphingosines

AUTHOR(S): Shibuya, Hirotaka; Kawashima, Keiko; Ikeda, Masahiko;

Kitagawa, Isao

CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, 565, Japan

SOURCE: Tetrahedron Lett. (1989), 30(51), 7205-8

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:131846

AB D-erythro-, L-erythro-, D-threo-, And L-threo-(E)-

HOCH2CH(NH2)CH(OH)CH:CH(CH2)12Me have been synthesized from

Z-butene-1,4-diol utilizing Sharpless asym. epoxidn. and a regiospecific ring-opening reaction of the resulting C4 chiral epoxide with an azide anion.

anion.

IT 2482-37-3P 128387-02-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and deacetylation of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 128387-02-0 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

IT 78779-96-1P 128387-01-9P 128387-05-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 128387-01-9 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R-[R*,S*-(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 128387-05-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R-[R*,R*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

L32 ANSWER 37 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1990:497937 CAPLUS

DOCUMENT NUMBER: 113:97937

TITLE: An efficient. stereoselective synthesis of 4-E- and Searched by Barb O'Bryen & Toby Port

4-Z-D-erythro-sphingenine and related compounds from

2-amino-2-deoxy-D-glucose

AUTHOR(S):

Sugawara, Tamio; Narisada, Masayuki

CORPORATE SOURCE:

Res. Lab., Shionogi and Co., Ltd., Osaka, 553, Japan

SOURCE:

Carbohydr. Res. (1989), 194, 125-38 CODEN: CRBRAT; ISSN: 0008-6215

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 113:97937

AB Efficient, stereoselective synthesis of 4-E- and 4-Z-D-erythrosphingenines having C16, C18, and C20 carbon-chains was achieved in 13 steps, starting from allyl 2-benzyloxycarbonylamino-2-deoxy-.alpha.-D-glucopyranoside. 2-Amino-1,6-di-O-tert-butyldiphenylsilyl-2-N-3-O-carbonyl-2-deoxy-D-allitol was used as the key intermediate.

IT 2482-37-3P 25494-35-3P 128387-01-9P

128745-57-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 25494-35-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 128387-01-9 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R-[R*,S*-(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 128745-57-3 CAPLUS

Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-, CN $[R-[R^*,S^*-(Z)]]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

L32 ANSWER 38 OF 72 CAPLUS COPYRIGHT 2000 ACS

1990:119279 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 112:119279

TITLE: Stereochemistry associated with the addition of

2-(trimethylsilyl)thiazole to differentially protected

.alpha.-amino aldehydes. Applications toward the

synthesis of amino sugars and sphingosines

AUTHOR (S): Dondoni, Alessandro; Fantin, Giancarlo; Fogagnolo,

Marco; Pedrini, Paola

CORPORATE SOURCE: Dip. Chim., Univ. Ferrara, Ferrara, Italy

J. Org. Chem. (1990), 55(5), 1439-46 SOURCE:

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

English LANGUAGE:

CASREACT 112:119279 OTHER SOURCE(S):

GI

AB The stereochem. and synthetic utility of the addn. of 2-(trimethylsilyl)thiazole (I) to various N-protected .alpha.-amino aldehydes is described. The reactions of I with N-Boc-L-serinal acetonide (BOC = tert-butoxycarbonyl) (II) and N-Boc-L-threoninal acetonide are essentially anti diastereoselective (ds = 85-90%) in agreement with the Felkin-Anh model for asym. induction, whereas the reactions with O-benzyl-NH-Boc-L-serinal and NH-Boc-L-phenylalaninal are syn diastereoselective (ds = 80%). The reversal of diastereoselectivity is interpreted on the basis of a proton-bridged cyclic Cram model for asym. induction. The anti adduct III (R = 2-thiazolyl) derived from II was subjected to thiazole-to-formyl unmasking to give a one-carbon higher homolog II (R = CHO). This material serves as a precursor to ribo- and arabino-4-amino-4-deoxypentoses via a further one-carbon-chain elongation with I and to a C20 sphingosine via Wittig olefination. The above ribo-amino sugar was transformed via sequential Wittig olefination and redn. into a C18 phytosphingosine. ΙT

25494-35-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 25494-35-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

L32 ANSWER 39 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1990:56573 CAPLUS

DOCUMENT NUMBER: 112:56573

TITLE: Preparation of sphingosine derivatives as antitumor

agents

INVENTOR(S): Sugimoto, Hirohiko; Sugawara, Tamio; Makino, Itsuo;

Sato, Kozaburo; Narisada, Masayuki

PATENT ASSIGNEE(S): Shionogi and Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 51 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01093562	A2	19890412	JP 1987-252276	19871005
TD 0500000		10070210		

JP 2588729 B2 19970312 OTHER SOURCE(S): MARPAT 112:56573

AB R1OCH2CHACH(OR2)CH:CH(CH2)nMe [I; R1 = H, acyl, glycosyl, phosphoric acid ester residue; R2 = H, acyl, glycosyl; A = (substituted) amino, N3; n = 10-14 integer], useful as antitumor agents and potentially useful for treatment of wounds and ulcers, are prepd. (2S,3R)-(Z)-HOCH2CH(NH2)CH(OH)CH:CH(CH2)12Me was acetylated with Ac2O to give (2S,3R)-(Z)-HOCH2CH(NHAC)CH(OH)CH:CH(CH2)12Me. In an in vivo study using MH 134 mouse tumor cells, 17 tested I at 2 mg i.p. showed 11->223% increase in life span of mice. About 40 I were prepd. with data.

IT 123446-95-7

RL: RCT (Reactant)

(reaction of, in prepn. of antitumor sphingosine derivs.)

RN 123446-95-7 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]meth yl]-3-heptadecenyl]-, [R-[R*,S*-(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

L32 ANSWER 40 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1990:36288 CAPLUS

DOCUMENT NUMBER: 112:36288

TITLE: Synthesis of D-erythro-1-deoxydihydroceramide-1-

sulfonic acid and phosphonosphingoglycolipid found in

marine organisms via a common precursor

AUTHOR(S): Ohashi, Kinji; Kosai, Shunji; Arizuka, Mitsuo;

Watanabe, Takashi; Yamagiwa, Yoshiro; Kamikawa, Tadao;

Kates, Morris

CORPORATE SOURCE: Fac. Sci. Technol., Kinki Univ., Higashi-Osaka, 577,

Japan

SOURCE: Tetrahedron (1989), 45(9), 2557-70

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 112:36288

GΙ

AB Galactopyranosylsphingosine deriv. I was prepd. from protected glycoside II in several steps. A sphingosine deriv. was converted to II.

IT 2482-37-3P

RN

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

2482-37-3 CAPLUS

CN Acetamide, N-[(1s, 2r, 3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-

heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

Searched by Barb O'Bryen & Toby Port

ΙI

L32 ANSWER 41 OF 72 CAPLUS COPYRIGHT 2000 ACS ACCESSION NUMBER: 1989:439825 CAPLUS

DOCUMENT NUMBER: 111:39825

TITLE: Unnatural ceramide-related compounds and their

preparation as intermediates for sphingoglycolipids

INVENTOR(S): Fujita, Shuji; Yoshimura, Shoji; Ito, Masayoshi;

Shitori, Yoshiyasu; Ogawa, Tomoya

PATENT ASSIGNEE(S): MECT Corp., Japan

SOURCE: Eur. Pat. Appl., 31 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	TENT NO.		KIND	DATE		API	PLICATION NO.	DATE
	293006 293006		A1 B1	19881130 19910612		EP	1988-108537	19880527
	R: AT,	BE, C	H, DE,	ES, FR,	GB,	GR,	IT, LI, LU, NL	, SE
JP	63297351	L	A2	19881205		JP	1987-132696	19870528
CA	1314052		A1	19930302		CA	1988-567227	19880519
IL	86487		A1	19920818		IL	1988-86487	19880525
UA	8816664		A1	19881201		AU	1988-16664	19880526
AU	608851		В2	19910418				
US	4880572		A	19891114		US	1988-199107	19880526
HU	46655		A2	19881128		HU	1988-2715	19880527
HU	200995		В	19900928				
DK	8802923		A	19881129		DK	1988-2923	19880527
FI	8802507		A	19881129		FI	1988-2507	19880527
ИО	8802342		A	19881129		NO	1988-2342	19880527
AΤ	64371		E	19910615		AT	1988-108537	19880527
HU	205894		В	19920728		HU	1990-3056	19880527
ES	2037763		Т3	19930701		ES	1988-108537	19880527
CN	1031077		A	19890215		CN	1988-103176	19880528
CN	1013440		В	19910807				
PRIORITY	APPLN.	<pre>INFO.:</pre>				JP	1987-132696	19870528
						EP	1988-108537	19880527

OTHER SOURCE(S): MARPAT 111:39825

GI

Unnatural ceramide related compds. (I and II; R1, R2 = OH, AcO, EtOCH2CH2O), useful as intermediates for sphingoglycolipids, were prepd., e.g. by deacylation of a benzylideneoctadecanediol deriv. (III). Thus, azidolysis 37.6%) of (2R, 3S)-1,3-O-benzylidene-2-O-methanesulfonyl-4-octadecene-1,2,3-triol with NaN3 in DMF at 100-110.degree., hydrogenation (38.8%) of the resulting (2S, 3S, 4E)- and (2S, 3S, 4Z)-2-azido-1,3-O-benzylidene-4-octadecene-1,3-diol over 10% Pd-C, and acylation (36.8%) of the product amine with lignoceric acid in the presence of 2-chloro-1-methylpyridinium iodide and Bu3N in CH2Cl2 gave III. Refluxing III in CH2Cl2-MeOH (1:1) contg. Amberlyst-15 gave 72.4% I (R1 = R2 = OH).

IT 121468-17-5P 121468-18-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, as intermediate for glycosphingolipids)

RN 121468-17-5 CAPLUS

CN Tetracosanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,R*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 121468-18-6 CAPLUS

CN Tetracosanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [S-[R*,R*-(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

Me (CH₂)₁₂
$$\overline{z}$$
 \overline{s} \overline{s} \overline{N} (CH₂)₂₂ \overline{s} \overline{s} \overline{N}

L32 ANSWER 42 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1989:8506 CAPLUS

DOCUMENT NUMBER: 110:8506

TITLE: A practical and enantioselective synthesis of

glycosphingolipids and related compounds. Total

synthesis of globotriaosylceramide (Gb3)

Ι

AUTHOR (S): Nicolaou, K. C.; Caulfield, T.; Kataoka, H.; Kumazawa,

Dep. Chem., Univ. Pennsylvania, Philadelphia, PA, CORPORATE SOURCE:

19104, USA

SOURCE: J. Am. Chem. Soc. (1988), 110(23), 7910-12

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 110:8506

GI

AB Glycosphingolipids were prepd. enantioselectively via prepn. of enantiomerically pure sphingosine equiv. I and its coupling to suitable carbohydrate donors utilizing the two-stage activation glycosidation procedure. This efficient method is demonstrated by the construction of galactosylceramide, lactosylceramide and Gb3, (II).

IT 2482-37-3P

> RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

2482-37-3 CAPLUS RN

CN Acetamide, N-[(1s,2r,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

L32 ANSWER 43 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1988:630620 CAPLUS

DOCUMENT NUMBER: 109:230620

TITLE: Synthesis of D-erythro- and D-threo-sphingosine

derivatives from L-serine

AUTHOR(S): Herold, Peter

CORPORATE SOURCE: Zent. Forschungslab., Ciba-Geigy A.-G., Basel,

CH-4002, Switz.

SOURCE: Helv. Chim. Acta (1988), 71(2), 354-62

CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:230620

GΙ

RN

The protected serine aldehyde I was converted to the title cryst.

N-protected sphingosines HOCH2CH(NHR)CH(OH)CH:CH(CH2)12Me [II, R = Me3CO2C (Boc)] by a three-step reaction sequence. I was transformed with high diastereoselectivity (95%) either to the erythro- or thero-alkynols III. erythro-III is formed by the addn. of LiC.tplbond.C(CH2)12Me in THF/HMP at -78.degree., whereas the corresponding thero-III is produced in the presence of ZnBr2 in Et2O. Deprotection of the acetal moiety afforded the corresponding 1,3-diols. These diols were selectively reduced with Red-Al to the (E)-sphingosines II, or the Z-isomers by partial hydrogenation over Lindlar's catalyst. Cleavage of the N-Boc group and further transformation to ceramides were readily achieved as demonstrated by the conversion of (E)-erythro-II (R = Boc) to N-octadecanoyl-D-erythro-sphingosine II [R = CO(CH2)16Me].

IT 2482-37-3P 78779-96-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

L32 ANSWER 44 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1988:590104 CAPLUS

DOCUMENT NUMBER: 109:190104

TITLE: Synthesis of D-erythro-1-deoxydihydroceramide-1-

sulfonic acid

AUTHOR(S): Ohashi, Kinji; Yamagiwa, Yoshiro; Kamikawa, Tadao;

Kates, Morris

CORPORATE SOURCE: Fac. Sci. Technol., Kinki Univ., Higashi-Osaka, Japan

SOURCE: Tetrahedron Lett. (1988), 29(10), 1185-8

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:190104

GΙ

- AB New D-erythro-1-deoxydihydroceramide-1-sulfonic acid (I), isolated from alkali-stable lipids in a non-photosynthetic marine diatom, Nitzschia alba, was synthesized from galactose as a chiral precursor using the reaction of acetal II with NBS-BaCO3 in CCl4 as the key step in the reaction sequence.
- IT 2482-37-3P

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3heptadecenyl]- (9CI) (CA INDEX NAME) Searched by Barb O'Bryen & Toby Port Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 45 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1988:549902 CAPLUS

DOCUMENT NUMBER: 109:149902

TITLE: Synthesis of a phosphonosphingoglycolipid found in the

marine snail Turbo cornutus

AUTHOR(S): Ohashi, Kinji; Kosai, Shunji; Arizuka, Mitsuo;

Watanabe, Takashi; Fukunaga, Mikio; Monden, Koji; Uchikoda, Takao; Yamagiwa, Yoshiro; Kamikawa, Tadao

CORPORATE SOURCE: Fac. Sci. Technol., Kinki Univ., Higashi-Osaka, Japan

SOURCE: Tetrahedron Lett. (1988), 29(10), 1189-92

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:149902

GΙ

CH₂OH NHCO (CH₂)₁₄Me
HO OCH₂CHCHCH=CH (CH₂)₁₂Me
OH
OH

AB The phosphonosphingoglycolipid I is synthesized from galactose as a chiral precursor via condensation of cerebroside II with

II

Ι

(HO) 2P(O) CH2CH2NMeCO2CH2CCl3 using EDCI as the key step.

IT 116448-00-1P

RN 116448-00-1 CAPLUS

CN Hexadecanamide, N-[1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-hydroxy-3-heptadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

L32 ANSWER 46 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1988:549173 CAPLUS

DOCUMENT NUMBER: 109:149173

TITLE: Asymmetric synthesis of threo- and

erythro-sphingosines by asymmetric aldol reaction of

.alpha.-isocyanoacetate catalyzed by a chiral

ferrocenylphosphine gold(I) complex

AUTHOR(S): Ito, Yoshihiko; Sawamura, Masaya; Hayashi, Tamio CORPORATE SOURCE: Dep. Synth. Chem., Kyoto Univ., Kyoto, 606, Japan

SOURCE: Tetrahedron Lett. (1988), 29(2), 239-40

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:149173

AB Asym. aldol reaction of CNCH2CO2Me with (E)-2-hexadecenal in the presence of 1 mol% of a chiral (aminoalkyl)ferrocenylphosphine-gold(I) complex gave optically active trans-4-(methoxycarbonyl)-5-[(E)-1-pentadecenyl]-2-

oxazoline which was readily converted into D-threo- and

erythro-sphingosines.

IT 116612-39-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and Mitsunobu reaction of)

RN 116612-39-6 CAPLUS

CN Acetamide, N-[1-[(acetyloxy)methyl]-2-hydroxy-3-heptadecenyl]-,
 [S-[R*,R*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

IT 2482-37-3P 78779-96-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1s, 2r, 3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-

heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

L32 ANSWER 47 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1988:510149 CAPLUS

DOCUMENT NUMBER: 109:110149

TITLE: A stereodivergent synthesis of D-erythro-sphingosine

and D-threo-sphingosine from L-serine

AUTHOR(S): Garner, Philip; Park, Jung Min; Malecki, Elise

CORPORATE SOURCE: Dep. Chem., Case West. Reserve Univ., Cleveland, OH,

44106-2699, USA

SOURCE: J. Org. Chem. (1988), 53(18), 4395-8

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:110149

GΙ

AB The stereocontrolled synthesis of both D-erythro-sphingosine I (R = OH, Rl= H) and D-threo-sphingosine I (R = H, Rl = OH) from L-serine-derived Searched by Barb O'Bryen & Toby Port

oxazolidine aldehyde II (Boc = CO2CMe3) is described. Addn. of LiC.tplbond.C(CH2)12Me to II proceeded with very good diastereoselectivity to give the erythro propargylic alc. III as expected for a non-chelated transition state. Redn. of III with lithium in ethylamine at -78.degree. resulted in clean redn. of the triple bond producing the protected sphingosine deriv. IV (R= OH, R1= H; V). Hydrolysis of this material with 1N HCl followed by extractive isolation and trituration led to the formation of I (R= OH, R1=H) in 65% overall yield from II. Prolonged exposure of V to lithium in ethylamine resulted in a novel fragmentation of the N-Boc oxazolidine moiety to give I directly in 68% overall yield after similar workup and recrystn. However, the addn. of (Me2CHCH2)2 AlCH:CH(CH2)12Me to II resulted in the moderately selective formation of threo allylic alc. IV (R= H, R1= OH) resulting from an .alpha.-chelation controlled transition state. This material was hydrolyzed with 1 N HCl to give a (2:1) mixt. of I (R, R1 = H, OH) in 60% overall yield.

IT 2482-37-3P 78779-96-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

L32 ANSWER 48 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1988:493486 CAPLUS

DOCUMENT NUMBER: 109:93486

TITLE: Stereoselective mono- and bis-homologation of

L-serinal via 2-(trimethylsilyl)thiazole addition.

Thiazole route to amino L-sugars and

D-erythro-sphingosines

AUTHOR(S): Dondoni, Alessandro; Fantin, Giancarlo; Fogagnolo,

Marco; Medici, Alessandro

CORPORATE SOURCE: Dip. Chim., Univ. Ferrara, Ferrara, Italy

SOURCE: J. Chem. Soc., Chem. Commun. (1988), (1), 10-12

CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 109:93486

GΙ

AB Anti-addn. [92% diastereoselectivity] of 2-trimethylsilylthiazole to O,N-protected L-serinal (I) and deblocking the formyl group in the resulting adduct, leads to the (2S,3S)-2,4-dihydroxy-3-aminobutanal deriv. (II), which serves as a precursor both to masked 4-amino-4-deoxy-L-ribose/L-arabinose and D-erythro-C2O-sphingosine.

IT 25494-35-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 25494-35-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

L32 ANSWER 49 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1987:420303 CAPLUS

DOCUMENT NUMBER: 107:20303

TITLE: Fumarase-catalyzed synthesis of L-threo-chloromalic

acid and its conversion to 2-deoxy-D-ribose and

D-erythro-sphingosine

AUTHOR(S): Findeis, Mark A.; Whitesides, George M.

CORPORATE SOURCE: Dep. Chem., Harvard Univ., Cambridge, MA, 02138, USA

SOURCE: J. Org. Chem. (1987), 52(13), 2838-48

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The use is described of pig heart fumarase (EC 4.2.1.2) as a catalyst in the multigram synthesis of L-threo-chloromalic acid (I) (.gtoreq.99.5% enantiomeric excess) on 50-g scale. L-threo-Fluoromalic acid has been synthesized in a coupled enzymic system from difluorofumaric acid. I serves as starting material for synthesis of 2-deoxy-D-ribose and D-erythro-sphingosine.

IT 2482-37-3P

RL: PREP (Preparation)

(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetvloxv)-1-[(acetvloxv)methvl]-3-Searched by Barb O'Bryen & Toby Port heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 50 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1986:626155 CAPLUS

DOCUMENT NUMBER: 105:226155

TITLE: Enantioselective synthesis of D-erythro-sphingosine

and of ceramide

AUTHOR(S): Julina, Radomir; Herzig, Thomas; Bernet, Bruno;

Vasella, Andrea

CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057,

Switz.

SOURCE: Helv. Chim. Acta (1986), 69(2), 368-73

CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 105:226155

GΙ

Me (CH₂) $_{12}$ CR = CR 1 CH (OH)

(E)-HC.tplbond.CCH:CHCH2OH was transformed into D-erythro-sphingosine in 7 AB steps and 46% overall yield and into ceramide in 8 steps and 41% overall yield. The key steps were the mono-epoxidn. of Me(CH2)12C.tplbond.CCH:CHCH2OH (by Ti(OCMe3)4, di-Et (-)-D-tartrate, and Me3COOH) to the (R,R)-epoxide (86%, .gtoreq.98% enantiomeric excess), the regioselective intramol. opening of the oxirane via the benzylurethane, and the reductive transformation of the acetylene I (RR1 = bond) into the oxazolidinone I (R = R1 = H).

TT 2482-37-3P

> RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

2482-37-3 CAPLUS

RN

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

CAPLUS COPYRIGHT 2000 ACS L32 ANSWER 51 OF 72

ACCESSION NUMBER: 1986:590762 CAPLUS

DOCUMENT NUMBER: 105:190762

TITLE: A novel, efficient synthesis of (.+-.)-erythro-

sphingosine

AUTHOR (S): Cardillo, Giuliana; Orena, Mario; Sandri, Sergio;

Tomasini, Claudia

CORPORATE SOURCE: Cent. Stud. Fis. Macromol., Ist. Chim. "G. Ciamician",

Bologna, 40126, Italy

Tetrahedron (1986), 42(3), 917-22 SOURCE:

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: English

CASREACT 105:190762 OTHER SOURCE(S):

In a stereoselective synthesis of (.+-.)-erythro-sphingosine triacetate AB (I) the key reaction that dets. the right stereochem. is the iodocyclization of (2E,4E)-Me(CH2)12(CH:CH)2CH2OC(:NH)CCl3 to the 4,5-dihydro-1,3-oxazine II. Cleavage of II with HCl and treatment with Amberlyst A 26 in the AcO- form, followed by full acetylation, affords I in good yield.

IT 86161-75-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 86161-75-3 CAPLUS

Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, CN

[R*,R*-(E)]-(9CI)(CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

L32 ANSWER 52 OF 72 CAPLUS COPYRIGHT 2000 ACS ACCESSION NUMBER: 1986:460459 CAPLUS

DOCUMENT NUMBER: 105:60459

TITLE: Synthesis of sphingosines. Part 2. Synthesis of

D-erythro-sphingosines

AUTHOR(S): Schmidt, Richard R.; Zimmermann, Peter

CORPORATE SOURCE: Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed.

Rep. Ger.

SOURCE: Tetrahedron Lett. (1986), 27(4), 481-4

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 105:60459

GΙ

AB 2,4-Di-O-protected D-threose, readily available from D-galactose, is a versatile intermediate for D-erythro-sphingosine, e.g., I, syntheses via trans-selective Wittig reaction, aside introduction at the unprotected hydroxylic group, and subsequent aside redn.

IT 25494-35-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

I

RN 25494-35-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

L32 ANSWER 53 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1986:221553 CAPLUS

DOCUMENT NUMBER: 104:221553

TITLE: Complete structural analysis of globoseries

glycolipids by two-dimensional nuclear magnetic

resonance

AUTHOR(S): Gasa, Shinsei; Nakamura, Mitsuru; Makita, Akira;

Ikura, Mitsuhiko; Hikichi, Kunio

CORPORATE SOURCE: Sch. Med., Hokkaido Univ., Sapporo, 060, Japan

SOURCE: Eur. J. Biochem. (1986), 155(3), 603-11

CODEN: EJBCAI; ISSN: 0014-2956

DOCUMENT TYPE: Journal

LANGUAGE: English

Combined 2-dimensional proton NMR allowed the detn. of complete AB oligosaccharide structures of glycolipids belonging to the globo series, without any other anal. methods. Although a chem. modification by peracetylation was required for the above purpose, the derivatization permitted facile assignment of the pyranose ring proton resonances of the oligosaccharide moiety. Two-dimensional chem.-shift-correlated spectroscopy of the acetylated glycolipid enabled elucidation the glycosidic positions from the chem. shifts of the protons at the substituted sites. The monosaccharide species were also identified from the characteristic splitting patterns of the methine protons on individual pyranose rings. The sequence of the monosaccharides was inferred from the interresidue connectivity across glycosidic linkages shown by 2-dimensional nuclear Overhauser effect spectroscopy, which also gave intraresidue interaction on the pyranose rings. The linkage sites of long oligosaccharide chains having more than 5 monosaccharides, such as globopentaosylceramide, were analyzed by 2-dimensional J-relayed coherence transfer, which yielded 1,3 interactions along with 1,2 interactions.

IT 2482-37-3

RL: PRP (Properties)
 (NMR spectrum of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 54 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1985:23726 CAPLUS

DOCUMENT NUMBER: 10:

TITLE: Diastereoselective synthesis of unsaturated vicinal

amino alcohols via Diels-Alder reactions of N-sulfinyl

dienophiles

AUTHOR(S): Garigipati, Ravi S.; Freyer, Alan J.; Whittle, Robert

R.; Weinreb, Steven M.

CORPORATE SOURCE: Dep. Chem., Pennsylvania State Univ., University Park,

PA, 16802, USA

SOURCE: J. Am. Chem. Soc. (1984), 106(25), 7861-7

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 102:23726

GI

AB .alpha.-Hydroxy-.beta.,.gamma.-unsatd. amine derivs. were synthesized from 3,6-dihydrothiazine 1-oxides, which were obtained stereoselectively by Diels-Alder [4 + 2] cycloaddn. of N-sulfinyl dienophiles and 1,3-dienes of known geometry. Fission of the S-N bond of the adduct with a Grignard reagent led to allylic sulfoxides which were converted stereoselectively to allyl alcs. via an allylic sulfoxide/sulfenate ester [2,3]-sigmatropic rearrangement. (E,E)- And (E,Z)-2,4-hexadiene were stereoselectively transformed to threo- and erythro-MeCH:CHCH(OH)CHMeNHCO2CH2Ph. Intermediates in these transformations were investigated by 1H NMR expts. The configuration and conformation of Diels-Alder adduct I were detd. by x-ray crystallog. and 1H NMR lanthanide induced shift expts. A variation of this strategy incorporating intramol. N-sulfinyl Diels-Alder reactions was used in the total synthesis of the sphingolipid bases erythro- (II) and threo-sphingosine.

IT 67113-24-0P 86161-75-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 67113-24-0 CAPLUS

CN Acetamide, N-[(1R,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry. Double bond geometry as shown.

RN 86161-75-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R*,R*-(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

L32 ANSWER 55 OF 72 CAPLUS COPYRIGHT 2000 ACS ACCESSION NUMBER: 1984:120758 CAPLUS

DOCUMENT NUMBER: 100:120758

Enantioselective synthesis of D-erythro-sphingosine TITLE:

Bernet, Bruno; Vasella, Andrea AUTHOR(S):

CORPORATE SOURCE: Org. Chem. Inst., Univ. Zurich, Zurich, CH-8057,

Switz.

SOURCE: Tetrahedron Lett. (1983), 24(49), 5491-4

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE:

Journal

English LANGUAGE:

D-erythro-Sphingosine [Me(CH2)12CH:CH(OH)CH(NH2)CH2OH, I] and the L-erythro isomer Me(CH2)12CH:CH(NH2)CH(OH)CH2OH were synthesized in a highly enantio- and regioselective manner by a modified Sharpless asym. epoxidn. The overall yield of I from CH.tplbond.C(CH2)12Me in 6 steps was 33%.

IT 89164-22-7P

> RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 89164-22-7 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, $[R-(R^*,S^*)]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

L32 ANSWER 56 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1983:438288 CAPLUS

DOCUMENT NUMBER: 99:38288

TITLE: Stereospecific synthesis of acyclic unsaturated amino

alcohols. A new approach to three and erythro

sphingosine

Garigipati, Ravi S.; Weinreb, Steven M. AUTHOR (S):

Dep. Chem., Pennsylvania State Univ., University Park, CORPORATE SOURCE:

PA, 16802, USA

SOURCE: J. Am. Chem. Soc. (1983), 105(13), 4499-501

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE:

Journal LANGUAGE: English

A new stereospecific synthesis of .alpha.-hydroxy-.beta.,.gamma.-unsatd. acyclic amines is based upon an initial stereospecific Diels-Alder cycloaddn. of PhCH2O2CN:SO with a 1,3-diene of known geometry, followed by conversion of the product to an allylic sulfoxide with PhMgBr. A stereospecific [2,3]-sigmatropic rearrangement of the allylic sulfoxide affords the desired unsatd. vicinal amino alc. This route has been applied to (E,E) and (E,Z)-MeCH:CHCH:CHMe to afford MeCH:CHCH(OH)CHMeNHCO2CH2Ph with total stereocontrol. The method has also been used in syntheses of threo- and erythro-sphingosine. A key strategy in these routes involves the first examples of intramol. N-sulfinyl-imine Diels-Alder processes.

IT 86161-75-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 86161-75-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, [R*,R*-(E)]-(9CI)(CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

L32 ANSWER 57 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1982:217554 CAPLUS

DOCUMENT NUMBER: 96:217554

TITLE: Diastereoselective synthesis of D,L-sphingosine

AUTHOR(S): Schmidt, Richard R.; Klaeger, Rudolf

CORPORATE SOURCE: Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed.

Rep. Ger.

SOURCE: Angew. Chem. (1982), 94(3), 215-16

CODEN: ANCEAD; ISSN: 0044-8249

DOCUMENT TYPE: Journal LANGUAGE: German

AB DL-Sphingosine was prepd. by reaction of Me(CH2)12CH:CHCHO with

(Me3Si)2NCH2CO2SiMe3 and LiAlH4 redn. of Me(CH2)12CH:CHCH(OH)CH(NH2)CO2H.

IT 67113-24-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(prepn. and deacetylation of)

RN 67113-24-0 CAPLUS

CN Acetamide, N-[(1R,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-

heptadecenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

L32 ANSWER 58 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1981:569690 CAPLUS

DOCUMENT NUMBER: 95:169690

TITLE: Useful syntheses of erythro- and threo-N-oleoyl-D-

sphingosines (ceramides) and galactosylceramides

(cerebrosides) from L-serine

AUTHOR(S): Tkaczuk, Peter; Thornton, Edward R.

CORPORATE SOURCE: Dep. Chem., Univ. Pennsylvania, Philadelphia, PA,

19104, USA

SOURCE: J. Org. Chem. (1981), 46(22), 4393-8

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: English

AB The 4-(carbomethoxy)-2-phenyl-.DELTA.2-oxazoline formed from L-serine is the basis for a useful synthesis of ceramides and cerebrosides on the 100 mg scale with .apprx.100% optical purity. The natural erythro configuration and its threo epimer. formed in equal amts.. are readily Searched by Barb O'Bryen & Toby Port

sepd. chromatog. so that both epimers are available for comparisons of the properties of erythro and threo configurations. The threo epimer and other analogs of the natural cerebrosides with different chain lengths and stereochem. should be readily available by this method.

IT 2482-37-3P 78779-96-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-

heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 78779-96-1 CAPLUS

CN Acetamide, N-[(1S,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

L32 ANSWER 59 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1978:442300 CAPLUS

DOCUMENT NUMBER: 89:42300

TITLE: Total synthesis of stereospecific sphingosine and

ceramide

AUTHOR(S): Shoyama, Yukihiro; Okabe, Hikaru; Kishimoto, Yasuo;

Costello, Catherine

CORPORATE SOURCE: John F. Kennedy Inst., Johns Hopkins Sch. Med.,

Baltimore, Md., USA

SOURCE: J. Lipid Res. (1978), 19(2), 250-9

CODEN: JLPRAW; ISSN: 0022-2275

DOCUMENT TYPE: Journal LANGUAGE: English

AB Et DL-erythro-2-acetamino-3-hydroxy-4-trans-octadecenoate was esterified with L(+)-acetylmandeloyl chloride and the two disastereomers obtained were sepd. from each other by thin-layer or column chromatog. One of the isomers was subjected to ethanolysis to obtain Et D-erythro-2-amino-3-

hydroxy-4-trans-octadecenoate which was then reduced with LiAlH4 or NaBH4 to yield D-erythro-sphingosine.

IT 2482-37-3P 67113-24-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetvloxv)-1-[(acetvloxv)methvl]-3-Searched by Barb O'Bryen & Toby Port heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 67113-24-0 CAPLUS

CN Acetamide, N-[(1R,2S,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3heptadecenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry. Double bond geometry as shown.

L32 ANSWER 60 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1977:38979 CAPLUS

DOCUMENT NUMBER:

86:38979

TITLE:

SOURCE:

Molecular arrangements in sphingolipids. Conformation

and hydrogen bonding of ceramide and their implication

on membrane stability and permeability

AUTHOR(S): Pascher, Irmin

CORPORATE SOURCE:

Fac. Med., Univ. Goteborg, Goteborg, Swed.

Biochim. Biophys. Acta (1976), 455(2), 433-51 CODEN: BBACAQ

DOCUMENT TYPE: Journal LANGUAGE: English

AB The preferred conformation of the ceramide part of sphingolipids was deduced from single crystal structures of a series of sphingolipid constituents: N-tetracosanoylphytosphingosine, glycosylphytosphingosine-HCl, sphingosine-HCl, triacetylsphingosine, DL-2-hydroxytetradecanoic acid, and N-stearoylethanolamine. The amide group of the ceramide, which serves as a link between the hydrocarbon chains, has a basic significance for the conformation of the entire mol. This rigid group, which comprises 6 atoms in a planar conformation, adopts a perpendicular orientation towards the axes of the 2 hydrocarbon chains. The carbonyl O thereby turns into an eclipsed position with the H atom at C-2 of the sphingosine. A parallel chain stacking is achieved by a sharp perpendicular bend of the fatty acid. This bend is produced by a sequence of 2 -60.degree. rotations about the C-C bonds at both sides of the .alpha.-C atom. orientation of the H bond donors and acceptors of the amide group and the hydroxyl groups allow lateral interaction with other lipid mols. The proposed models are supported by IR spectra, thin-layer chromatog. behavior, and monolayer studies of synthetic model ceramides. The functional role of the H bonding groups in the ceramide part of sphingolipids is emphasized and their significance for the formation of lateral H bonds within the membrane layer and thereof arising effects on membrane stability and permeability are discussed. Searched by Barb O'Bryen & Toby Port

IT 25494-35-3

RL: PRP (Properties)

(crystal structure of, ceramide conformation in relation to)

RN 25494-35-3 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-,

 $[R-[R^*,S^*-(E)]]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

L32 ANSWER 61 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1976:150300 CAPLUS

DOCUMENT NUMBER:

84:150300

TITLE:

Synthesis of sphingomyelins via their dimethylamino

precursors

AUTHOR(S):

Zvonkova, E. N.; Mitsner, B. I.; Bushnev, A. S.;

Orlova, E. G.; Gabor, Kruppa; Markina, N. N.;

Talagaeva, S. V.; Evstigneeva, R. P.

CORPORATE SOURCE:

M. V. Lomonosov Inst. Fine Chem. Technol., Moscow,

USSR

SOURCE:

Bioorg. Khim. (1975), 1(12), 1746-54

CODEN: BIKHD7

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

AB Sphingomyelins, based on trimethylammonio derivs. of sphingenine, rac-sphinganine, and threo-rac-sphinganine were prepd. 3-Benzoylceramide phosphoryldimethylaminoethyl derivs. were prepd. from 3-benzoylceramides via 2-chloroethylphosphoryl-3-benzoylceramides or 3-benzoylceramide phosphates. The 3-benzoylceramide prepn. was modified, and

3-benzoyl-rac-sphingenine sulfate was resolved with d-(+)-tartaric acid.

IT 2482-37-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S, 2R, 3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-

heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 62 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1975:116603 CAPLUS

DOCUMENT NUMBER: 82:116603

TITLE: Monolaver studies on derivatives of sphinganine and

4t-sphingenine

AUTHOR(S):

Stoffel, W.; Pruss, H. D.; Sticht, G.

CORPORATE SOURCE:

Inst. Physiol. Chem., Univ. Koeln, Cologne, Ger.

SOURCE:

Chem. Phys. Lipids (1974), 13(4), 466-80

CODEN: CPLIA4

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB The pressure-area isotherms at 4-47.degree. of the following derivs. of sphinganine and 4t-sphingenine were detd.; N-palmitoyl-D,L-sphingenine (I), N-palmitoyldiacetyl-D, L-sphingenine (II), N-acetylsphingenine (III), N-acetyl-D, L-erythro-sphinganine (IV), N-acetyl-D, L-threo-sphinganine (V), triacetyl-D, L-erythro-sphinganine (VI), N-acetyl-3-dehydrosphingenine (VII), N-acetyl-3-dehydro-D,L-sphinganine (VIII) and diacetyl-3-dehydro-D, L-sphinganine (IX). The phases of the monolayer films are discussed. III, V, VI, VIII, and IX form trilayers when their monolayers are compressed beyond the collapse point. The folding to a trilayer is only possible from the liq. expanded state of the monolayer. The formation of trilayer films occur only when the area of the hydrophilic group exceeds that of the alkane chain of the long chain base.

IT 54824-82-7

RL: PRP (Properties)

(monolayers of)

RN 54824-82-7 CAPLUS

CN Hexadecanamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]-, $[R^*, S^*-(E)]-(9CI)$ (CA INDEX NAME)

Relative stereochemistry. Double bond geometry as shown.

ACO
$$R$$
 E $CH_2)_{14}$ NH $CCH_2)_{14}$ NH $CCH_2)_{14}$ NH

L32 ANSWER 63 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER:

1973:432244 CAPLUS

DOCUMENT NUMBER:

79:32244

TITLE:

Structural studies on glycolipids. 1. 220 MHz PMR

spectra of acetylated galactocerebrosides

AUTHOR(S):

Martin-Lomas, M.; Chapman. D.

CORPORATE SOURCE:

Biophys. Div., Unilever Res. Lab., Welwyn/Herts.,

Engl.

SOURCE:

Chem. Phys. Lipids (1973), 10(2), 152-64

CODEN: CPLIA4

DOCUMENT TYPE:

Journal

LANGUAGE:

English

The PMR spectra of fully acetylated 2-amino-trans-2S, 3R-4-octadecene-1, 3diol (sphingosine), the dihydro deriv., 1-0-.beta.-D-galactopyranosyl-2tetracosanoylamido-trans-2S, 3R-4-octadecene-1, 3-diol (cerasine), and 1-0-.beta.-D-galactopyranosyl-2-hydroxy-2-tetracosanoylamido-trans-2S,3R-4octadecene-1,3-diol (phrenosine) were detd. in CDCl3, CD3COCD3 and benzene-d6 at 220 MHz. The relative chem. shifts of the protons in the three solvents permitted configurational and conformational detns.

ΙT 2482-37-3

RL: RCT (Reactant)

(PMR of, configuration in relation to)

2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 64 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER:

1973:68524 CAPLUS

DOCUMENT NUMBER:

78:68524

TITLE:

RN

Carbon-13-nuclear magnetic resonance spectroscopic

studies on saturated, mono-, di-, and polyunsaturated

fatty acids, phospho- and sphingolipids

AUTHOR (S):

Stoffel, Wilhelm; Zierenberg, Ottfried; Tunggal, Budi

D:

CORPORATE SOURCE:

SOURCE:

Inst. Physiol. Chem., Univ. Koeln, Cologne, Ger.
Hoppe-Seyler's Z. Physiol. Chem. (1972), 353(12),

1962-9

Journal

CODEN: HSZPAZ

DOCUMENT TYPE:

LANGUAGE:

English

AB Complete and unequivocal 13C magnetic resonance data have been obtained for the following biol. relevant lipids: the fatty acids palmitic, stearic, oleic, linoleic, .alpha.-linolenic, and arachidonic acids; the phospholipids 1-stearoyl-2-linoleoyl-3-glycerophosphorylcholine. 1,2-Distearoyl-3-glycrophosphorylcholine, phosphatidylcholine-choline-N-methyl-13C, sphingomyelin-choline-N-methyl-13C; sphinganine (dihydrosphingosine), 4t-sphingenine (sphingosine), and 3-dehydrospinganine. Accurate assignments of resonance lines were ascertained using synthetic compds. labeled with .apprx.90% 13C in specific positions of the resp. mol. and substituted differentially. The parameters detg. the chem. shifts were analyzed.

IT 40747-69-1

RL: PRP (Properties)

(NMR of)

RN 40747-69-1 CAPLUS

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl-3-t]-, $[R-[R^*,S^{*-}(E)]]- (9CI) \quad (CA \ INDEX \ NAME)$

Absolute stereochemistry.

Double bond geometry as shown.

L32 ANSWER 65 OF 72 CAPLUS COPYRIGHT 2000 ACS ACCESSION NUMBER: 1972:127356 CAPLUS

DOCUMENT NUMBER: 76:127356

TITLE: Molecular arrangements in glycosphingolipids

AUTHOR(S): Abrahamsson, Sixten; Pascher, Irmin; Larsson, Kare;

Karlsson, Karl A.

CORPORATE SOURCE: Swed. Med. Res. Counc. Unit Mol. Struct. Anal., Univ.

Goteborg, Goteborg, Swed.

SOURCE: Chem. Phys. Lipids (1972), 8(2), 152-79

CODEN: CPLIA4

DOCUMENT TYPE: Journal LANGUAGE: English

Homogeneous glycosphingolipids are prepd. and their structural behavior studied in the solid state as well as in lipid-water systems and in surface films. Mainly x-ray diffraction techniques are used in the phase anal. A very complex phase pattern is usually found-e.g., cerebroside contg. 2-hydroxy fatty acids has 5 cryst. phases and 2 thermotropic mesophases. This is also the case in the water systems, where hexagonal, lamellar, and cubic mesophases are obsd. Whereas in earlier surface film studies of complex lipids, such as phospholipids, only one liq. expanded phase usually has been found, cerebrosides also exhibit numerous condensed phases. Comparisons with corresponding natural lipids show a close relation both in the phase behavior and structure of the different polymorphs.

IT 2482-37-3

RL: PROC (Process)

(structural behavior of, in solid liq. and soln. states)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L32 ANSWER 66 OF 72 CAPLUS COPYRIGHT 2000 ACS ACCESSION NUMBER: 1971:485024 CAPLUS

DOCUMENT NUMBER: 75:85024

TITLE: Thin-layer chromatography of ceramides

AUTHOR(S): Karlsson, Karl L.; Pascher, Irmin

CORPORATE SOURCE: Dep. Med. Biochem., Univ. Goteborg, Goteborg, Swed.

SOURCE: J. Lipid Res. (1971), 12(4), 466-72

CODEN: JLPRAW

DOCUMENT TYPE: Journal LANGUAGE: English

AB Ceramides with mono-, di-, and trihydroxy long-chain bases, and normal (satd. and unsatd.), branched-chain, and 2-hydroxy fatty acids were analyzed by thin-layer chromatog. In most cases the compds. were also run as acetates. Borate, arsenite, and Ag+ were used as complexing agents, and the effects of no., position, and stereochemistry of OH groups, and of unsatn., were studied. The results are discussed in view of anal. of natural ceramide species.

IT 2482-37-3 34227-61-7 34249-35-9

34249-37-1 34435-03-5

RL: ANT (Analyte); ANST (Analytical study)
 (chromatog. of)

RN 2482-37-3 CAPLUS

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 34227-61-7 CAPLUS

CN Linoleamide, N-[2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-, diacetate (ester), (E)-D-erythro- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Me (CH₂)
$$\frac{1}{2}$$
 E $\frac{1}{2}$ CH₂) $\frac{1}{4}$ Me OAC

RN 34249-35-9 CAPLUS

CN Octadecanamide, N-[2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-, diacetate (ester), (E)-D-erythro- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 34249-37-1 CAPLUS

CN Oleamide, N-[2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-, diacetate (ester), (E)-D-erythro- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Me} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

34435-03-5 CAPLUS RN

CN Tetracosanamide, N-[2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-, diacetate (ester), (E)-D-erythro- (8CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

L32 ANSWER 67 OF 72 CAPLUS COPYRIGHT 2000 ACS

1970:99972 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 72:99972

TITLE: Lipids. Synthesis of C20-sphingosine

Zvonkova, E. N.; Vlakhliiska, T. D.; Soldatova, S. A.; AUTHOR (S):

Mitsner, B. I.; Preobrazhenskii, N. A.

CORPORATE SOURCE: Mosk. Inst. Tonkoi Khim. Tekhnol. im. Lomonosova,

Moscow, USSR

Zh. Org. Khim. (1970), 6(1), 58-62 SOURCE:

CODEN: ZORKAE

DOCUMENT TYPE: Journal LANGUAGE: Russian

Condensation of 2-trans-octadecenyl chloride with AcCHNaCO2Et gave AB Me(CH2)14CH:CHCOCHAcCO2Et (I). I with PhN2+Cl- in a buffered soln. gave

Me(CH2)14CH:-CHCOC(:NNPh)CO2Et which was reduced with Zn/AcOH to Me(CH2)14CH:CHCOCH(NHAc)CO2Et (II). Redn. of II with NaBH4 gave

Me(CH2)14CH:CHCH(OH)CH(NHAc)CO2Et (III) (2 isomers sepd. by fractional crystn.). Deacetylation of erythro-III gave Me(CH2)14CH:CHCH(OH)CH(NH2.HC 1) CO2Et, which was reduced with LiAlH4 to C20-sphingosine, which was

Searched by Barb O'Bryen & Toby Port

addnl. characterized as Me(CH2)14CH:CHCH(OAc)CH(NHAc)CH2OAc.

IT 25494-35-3P

> RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

 $[R-[R^*,S^*-(E)]]-(9CI)$ (CA INDEX NAME)

25494-35-3 CAPLUS

RN CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-,

Absolute stereochemistry. Double bond geometry as shown.

L32 ANSWER 68 OF 72 CAPLUS COPYRIGHT 2000 ACS

1970:48667 CAPLUS ACCESSION NUMBER:

72:48667 DOCUMENT NUMBER:

Crystal structure of triacetylsphingosine TITLE:

AUTHOR(S): O'Connell, A. M.; Pascher, I.

CORPORATE SOURCE: Med. Res. Counc. Unit, Univ. Goteborg, Goteborg, Swed.

Acta Crystallogr., Sect. B (1969), 25(Pt. 12), 2553-61 SOURCE:

CODEN: ACBCAR

DOCUMENT TYPE: Journal English LANGUAGE:

The crystal structure of triaceyl-sphingosine (D-erythro-1,3-diacetoxy-2acetamido-4-trans-octadecene, C24H43O5N) has been detd. by direct methods. The crystals are orthorhombic, P212121, with a 5.002, b 8.709, and c 60.62 .ANG.. Positional and isotropic thermal parameters of the non-H atoms were refined to give a final R index of 0.109. The mols. are arranged head-to-tail in layers within which the C chains pack according to the common orthorhombic subcell, O .perp.. The chain axis forms an angle of 58.degree. with the end group planes. Adjacent layers show opposite tilt of the chains. In spite of the bulky acetyl branches, the mols. adopt a very effective packing (dm = 1.07). The mols. are connected by a continuous system of N-H-O hydrogen bonds parallel to a, and there is also evidence for 2 weaker C-H-O type interactions.

2482-37-3 IT

> RL: PRP (Properties) (crystal structure of)

RN 2482-37-3 CAPLUS

Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-CN heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

CAPLUS COPYRIGHT 2000 ACS L32 ANSWER 69 OF 72

ACCESSION NUMBER: 1969:509739 CAPLUS

DOCUMENT NUMBER: 71:109739

TITLE: Preparation of ceramides from brain gangliosides and

the nature of the sphingosine bases

AUTHOR (S): Klenk, Ernst; Huang, Richard T. C.

CORPORATE SOURCE: Univ. Koeln, Cologne, Ger.

SOURCE: Hoppe-Seyler's Z. Physiol. Chem. (1969), 350(9),

1081-7

CODEN: HSZPAZ

DOCUMENT TYPE:

LANGUAGE:

German

AB Ganglio-ceramides were prepd. in practically quant. yield from brain gangliosides, following oxidn. with periodate, redn. with NaBH4, and mild acid hydrolysis. The mixt. of sphingosine bases obtained from them was sepd. into its individual components by the counter-current distribution of the triacetyl compds.; the triacetyl deriv. of C20-sphingosine was isolated for the first time. The yield was 40% of the original mixt. of the sphingosine bases. The properties of the isolated substance agree with the structure D-erythro-1,3-dihydroxy - 2-amino-trans-4-eicosene.

IT 25494-35-3

> RL: ANST (Analytical study) (from gangliosides, of brain)

RN 25494-35-3 CAPLUS

Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-nonadecenyl]-, CN $[R-[R^*,S^*-(E)]]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

L32 ANSWER 70 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1968:48956 CAPLUS

DOCUMENT NUMBER: 68:48956

TITLE: Metabolism of sphingosine bases. III. Chemical syntheses of carbon-14 and tritium labeled erythro-

and threo-dihydrosphingosines and sphingosines

AUTHOR(S): Stoffel, Wilhelm; Sticht, Guido

Univ. Cologne, Cologne, Ger. CORPORATE SOURCE:

Hoppe-Seyler's Z. Physiol. Chem. (1967), 348(12), SOURCE:

1561-9

CODEN: HSZPAZ

DOCUMENT TYPE:

Journal LANGUAGE: English

Labeled sphingosines and dihydrosphingosines were prepd. for use in biochem. research. Acrolein was brominated in ether to give 2,3-dibromopropanal, whose di-Et, acetal (I), b13 108-12.degree., n20D 1.4969, was formed by treatment with HC(OEt)3 and EtOH. I was dehalogenated with NaNH2 in liq. NH3, giving propynal di-Et acetal (II), b760 138-40.degree. and n20D 1.4141. LiC.tplbond.CCH(OEt)2 was then formed in NH3 from II and treated with 1-bromotridecane, giving 2-hexadecyne-1-al di-Et acetal (III), b0.01125.degree., n20D 1.4490. was catalytically reduced in an amt. of 3H, giving palmitaldehyde-2,2,3,3t4 di-Et acetal, which by acid hydrolysis with simultaneous complete exchange of .alpha.-protons gave palmitaldehyde-3,3-t2 (IV), b0.1 125-30.degree., sp. activity 31.2 .mu.Ci./.mu.mole. Condensing IV with nitroethanol gave .apprx.13-17% thero-2-nitrooctadecan-1,3-diol (V), m. 81-2.5.degree., and a mixt. (A) of threo and erythro-isomers, m. 38.degree.. threo-DL-Dihydrospingosine-5,5-t2 (VI), m. 93-5.degree., was prepd. by reducing I with Al amalgam in Et20. The triacetyl deriv. of VI m. 66.5.degree.. A was treated with BzH and ZnCl2, giving erythro-5-nitro-4-pentadecyl-(2,2-t2)-1,3-dioxane, m. 49.degree., which was reduced with Al amalgam to the 5-amino compd., m. 47-9.degree.. This compd. was acetylated with Ac20 in pyridine, giving the N-acetyl deriv., m. 131.degree.. Hydrolvsis with HCl in dioxane gave ervthro-DL-Searched by Barb O'Bryen & Toby Port

dihydrosphingosine-5,5-t2, m. 83.degree., triacetyl deriv. m. 91-2.degree.. The racemate of VI was sepd. into optical antipodes via the L-glutamate, giving the threo-(+)-L-dihydrosphingosine. The C-acylation of Na acetoacetate by the method of Helferich gave Et 2-acetyl-3oxooctadecanoate-3-14C, which gave the 2-phenylhydrazone by the Japp-Klingemann reaction. Treatment with Zn in HCO2H gave the 2-amino compd. (VII), m. 122-4.degree.. The LiAlH4 redn. of the 3-oxo group gave the desired erythro- and threo-dihydrosphingosines-3-14C. The diastereomeric mixt. was transformed into the N-dichloroacetyl deriv. and the cryst. erythro form, m. 138.degree., was hydrolyzed to give the free pure erythro compd., m. 83-4.degree.. The LiAlT4 redn. of IV, followed by isomer sepn. as before, gave the erythro-DL-dihydrosphingosine-1,1-t2-3-14C, m. 84.5.degree.. 2-Tetradecyn-1-al di-Et acetal, b0.1 138-45.degree., was prepd. as above, and hydrogenated with 3H to give myristaldehyde-3,3-t2. Condensation with malonic acid gave hexadecanoic-5,5-t2 acid, m. 49.degree., which was converted to the chloride, b0.005 135.degree., n25D 1.4644. Et 2-acetyl-3-oxooctadecenoate-7,7-t2, m. 35.degree., and the phenylhydrazone of Et 2,3-dioxo-4-transoctadecenoate-7,7-t2, m. 54-6.degree., Et 2-acetamido-3-oxo-4-transoctadecenoate-7,7-t2, m. 65.degree., Et 2-acetamido-3-hydroxy-4-transoctadecenoate-7,7-t2, m. 56.degree., and Et 2-amino-3-hydroxyoctadecenoate-7,7-t2 hydrochloride, m. 108-10.degree., were prepd. by previously given methods. The latter compd. was reduced with LiAlH4, giving erythro-DL-sphingosine-7,7-t2, m. 67.degree., triacetyl deriv. m. 89.5.degree.. 21300-78-7P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of) 21300-78-7 CAPLUS L32 ANSWER 71 OF 72 CAPLUS COPYRIGHT 2000 ACS 1967:508121 CAPLUS ACCESSION NUMBER: DOCUMENT NUMBER: 67:108121 Synthesis of DL-erythro and threo-sphingosine-4,5-3H TITLE: AUTHOR(S): Gal, Andrew E. Natl. Inst. of Neurological Diseases and Blindness, CORPORATE SOURCE: Natl. Inst. of Health, Bethesda, Md., USA J. Labelled Compd. (1967), 3(2), 112-19 SOURCE: CODEN: JLCAAI DOCUMENT TYPE: Journal LANGUAGE: English DL-erythro-Sphingosine (Ia) and DL-threo-sphingosine (II) [Me(CH2)12CH:CH(OH)CH(NH2)CH2OH] specifically labeled with 3H in positions 4 and 5 were prepd. The synthesis of these compds. was based on a modification of a procedure by Grob and Gadient (CA 52: 7202h). Quant. sepn. of the sphingosines from acetylenic impurities was accomplished, and the phys. consts. of pure I and II were detd. I was prepd. by resolving the DL racemate and it was identical to the naturally occurring product. 16 references. 2482-37-3P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of) 2482-37-3 CAPLUS Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3heptadecenyl] - (9CI) (CA INDEX NAME)

IT

RN

ΙT

RN

CN

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

L32 ANSWER 72 OF 72 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1967:481783 CAPLUS

DOCUMENT NUMBER: 67:81783

TITLE: Sphingolipids. II. Synthesis of ceramide-like

compounds

AUTHOR(S): Auer, E.; Libert, Hermann; Schmid, Leopold

CORPORATE SOURCE: Univ. Vienne, Vienna, Austria

SOURCE: Monatsh. Chem. (1967), 98(3), 802-6

CODEN: MOCHAP

DOCUMENT TYPE: Journal LANGUAGE: German

AB cf. CA 67: 2727z. DL-threo-Me(CH2)12C.tplbond.CCH(OH)CH(NH2)CH2OH was hydrogenated using Lindlar catalyst at 20.degree. to give 90% DL-threo-cis-Me(CH2)12CH:CHCH(OH)CH(NH2)CH2OH(I). I gave by further hydrogenation 82% DL-threo-Me(CH2)14CH(OH)CH(NH2)CH2OH, m. 98-100.degree.. I (1 g.) in 20 ml. HCONMe2 and 0.3 ml. dry pyridine was treated with 1.3 q. liqnoceric acid chloride in 15 ml. HCONMe2 to give DL-threo-cis-Me(CH2)12CH:CHCHRCH[NHCO(CH2)22Me]CH2R'(II) (R = R' = OH) (III), m. 100-2.degree.. Similarly was prepd. DL-threo-cis-Me(CH2) 12CH: CHCHRCH[NHCO(CH2) 12Me) CH2R' (IV) (R = R' = OH), m. 96.5-98.degree.. III in tetrahydrofuran and pyridine treated with 0.6 g. Ph3CCl gave 67% II (R = OH, R' = OCPh3). Similarly was prepd. IV (R = OH, R' = OCPh3) in 79% yield. II (R = OAc, R' = OCPh3), II (R = OAc, R' = OAc) OH), (m. 95.5-97.degree.), IV (R = OAc, R' = OCPh3), and IV (R = OAc, R' = OAc,OH) (m. 93-5.degree.) were prepd. as usual. II (R = R' = OAc), m. 67-8.degree., was prepd. in 75% yield from III by acetylation.

IT 17673-77-7P

RN 17673-77-7 CAPLUS

CN Tetracosanamide, N-[2-hydroxy-1-(hydroxymethyl)-3-heptadecenyl]-, diacetate (ester), (Z)-DL-threo- (8CI) (CA INDEX NAME)

Relative stereochemistry. Double bond geometry as shown.

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Searched by Barb O'Bryen & Toby Port

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L2
                STR
L3
                STR
L4
            983 SEA FILE=REGISTRY SSS FUL L2 NOT L3
L7
                STR
            650 SEA FILE=REGISTRY SUB=L4 SSS FUL L7
T-10
L28
                STR
T.31
             46 SEA FILE=REGISTRY SUB=L10 SSS FUL L28
L33
             13 SEA FILE=CAOLD ABB=ON PLU=ON L31
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L33 ANSWER 1 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA65:17257g CAOLD

TITLE: phys. studies of phospholipids - (IV) high resolution

nuclear magnetic resonance spectra of phospholipids and

related substances

AUTHOR NAME: Chapman, Dennis; Morrison, A.

TITLE: properties of phosphatides prepd. from rice bran and

Phaseolus aureus

AUTHOR NAME: Talwalkar, R. T.; Garg, N. K.; Krishna Murti, C. R.

INDEX TERM: 67-48-1 102-76-1 122-32-7 555-43-1 816-93-3

1071-23-4 2462-63-7 **2482-37-3** 3338-29-2

4826-71-5 5683-50-1 5683-54-5 7768-08-3 14479-96-0

14672-00-5 14834-15-2 15557-11-6 16777-83-6

96579-26-9 106065-93-4 106571-73-7

IT 2482-37-3 96579-26-9

RN 2482-37-3 CAOLD

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 96579-26-9 CAOLD

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

L33 ANSWER 2 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA62:9754e CAOLD

TITLE: sepn. of long-chain bases by thin-layer chromatography-

instability of sphingosine

AUTHOR NAME: Weiss, Benjamin; Stiller, R. L.

INDEX TERM: 123-78-4 764-22-7 992-35-8 2304-74-7 2304-75-8

2304-76-9 2304-77-0 2304-78-1 2304-80-5 2304-81-6

2304-82-7 2458-06-2 **2482-37-3** 2673-72-5

2675-54-9 2675-55-0 2675-56-1 2675-57-2 2872-63-1

30684-99-2 38107-88-9 54336-64-0 94381-13-2 94381-57-4

95423-51-1 **96579-26-9** 96673-02-8 96772-09-7

96772-16-6

IT 2482-37-3 96579-26-9

RN 2482-37-3 CAOLD

CN Acetamide, N-[(1S,2R,3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 96579-26-9 CAOLD

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

L33 ANSWER 3 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA62:6843a CAOLD

TITLE: structural components of the pvridine-insol. sphingolipid Searched by Barb O'Bryen & Toby Port

from Corbicula sandai, and the distribution in other species

AUTHOR NAME: Hori, Taro; Itasaka, O.; Inoue, H.; Yamada, K. INDEX TERM: 501-11-1 2041-14-7 2461-23-6 2482-37-3

7518-10-7 **96579-26-9**

IT 2482-37-3 96579-26-9

RN 2482-37-3 CAOLD

CN Acetamide, N-[(1S, 2R, 3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-

heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 96579-26-9 CAOLD

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

L33 ANSWER 4 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA58:12407b CAOLD

TITLE: action of esters of chlorosulfurous acid on alkyl

sulfates-prepn. of diethyl sulfate

AUTHOR NAME: Kraft, M. Ya.; Lyutina, F. V.

INDEX TERM: 24028-07-7 96770-39-7

IT 96770-39-7

RN 96770-39-7 CAOLD

CN Acetamide, N-[2-hydroxy-1-(hydroxymethyl)-3-nonadecenyl]-, diacetate (7CI) (CA INDEX NAME)

L33 ANSWER 5 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA58:11370g CAOLD

TITLE: sphingosine, stereospecific syntheses of compds. related to

PATENT ASSIGNEE: CIBA Ltd.

DOCUMENT TYPE: Patent

PATENT NO. KIND DATE

PI GB 864261

INDEX TERM: 13552-54-0 94375-81-2 94676-99-0 95220-02-3

96579-26-9 97258-24-7 97282-27-4 97282-28-5

101635-19-2

IT 96579-26-9

RN 96579-26-9 CAOLD

Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) CN (CA INDEX NAME)

AcNH OAc $AcO-CH_2-CH-CH-CH-CH-CH-(CH_2)_{12}-Me$

L33 ANSWER 6 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA55:23611f CAOLD

effect of mevalonate analogs on cholesterol biosynthesis TITLE:

Weiss, Herbert; Schiffman, E.; Titus, E. O. AUTHOR NAME:

INDEX TERM: 13552-09-5 **96579-26-9**

IT 96579-26-9

RN 96579-26-9 CAOLD

Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) CN (CA INDEX NAME)

ACNH OAC $Aco-Ch_2-Ch-Ch-Ch-Ch-Ch-Ch-Ch_1-Ch-Ch_2$

L33 ANSWER 7 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA55:19796c CAOLD

2,2,4,6,6-pentachloro-5-oxo-3-hexenoic acid esters TITLE:

PATENT ASSIGNEE: Ruhrchemie Akt.-Ges.

DOCUMENT TYPE: Patent

esters of 2,2,4,6,6-pentachloro-5-oxo-3-hexenoic acid TITLE:

AUTHOR NAME: Feichtinger, Hans; Puschhof, S.

DOCUMENT TYPE: Patent

> PATENT NO. KIND DATE ______ _____

PΙ DE 1056119

INDEX TERM: 13552-54-0 **96579-26-9** 108128-78-5 108128-79-6

114379-89-4 117882-92-5

IT 96579-26-9

RN 96579-26-9 CAOLD

Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) CN (CA INDEX NAME)

AcNH OAc $AcO-CH_2-CH-CH-CH=CH-(CH_2)_{12}-Me$

L33 ANSWER 8 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA55:19795e CAOLD

TITLE: 1,3-dihydroxy-2-amino-4-alkenes, stereospecific method for

the prepn. of

PATENT ASSIGNEE: CIBA Ltd.

DOCUMENT TYPE: Patent

TITLE: prepn. of 1,3-dihydroxy-2-amino-4-alkenes

AUTHOR NAME: Grob, Cyril A.

DOCUMENT TYPE: Patent

> PATENT NO. KIND

PΙ DE 1070168

INDEX TERM:

13552-54-0 94375-81-2 94676-99-0 95220-02-3

96579-26-9 97258-24-7 101635-19-2 114697-01-7

96579-26-9 IT

RN 96579-26-9 CAOLD

Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) CN (CA INDEX NAME)

AcNH OAc $AcO-CH_2-CH-CH-CH-CH-CH-(CH_2)_{12}-Me$

L33 ANSWER 9 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA53:14930f CAOLD

TITLE:

marine products - (XLVII) phospholipides of a sea anemone

AUTHOR NAME:

Bergmann, Werner; Landowne, R. A.

TITLE:

prepn., purification, and characterization of amino acid

derivs. of ethanolamine

AUTHOR NAME:

Smith, Elizabeth C.

INDEX TERM:

536-14-1 **2482-37-3** 105976-74-7

IT 2482-37-3

RN 2482-37-3 CAOLD

CN Acetamide, N-[(1s, 2r, 3E)-2-(acetyloxy)-1-[(acetyloxy)methyl]-3-

heptadecenyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

OAc $(CH_2)_{12}$ Aco NHAc

L33 ANSWER 10 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA52:13632e CAOLD

TITLE:

total synthesis of sphingosine

AUTHOR NAME: INDEX TERM:

Shapiro, David; Segal, H.; Flowers, H. M. 629-56-1 6491-57-2 7369-94-0 13477-50-4 40514-39-4

96579-26-9 101726-30-1 102464-85-7 102944-39-8

102944-67-2 103044-18-4

IT 96579-26-9

RN 96579-26-9 CAOLD

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) (CA INDEX NAME)

ACNH OAC $Aco-Ch_2-Ch-Ch-Ch-Ch-Ch-(Ch_2)_{12}-Me$

L33 ANSWER 11 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA52:7202h CAOLD

TITLE:

synthesis of sphingosine and its stereoisomers

AUTHOR NAME:

Grob, Cyril A.; Gadient, F.

INDEX TERM:

765-09-3 765-13-9 13552-12-0 13552-54-0 18696-97-4

51534-40-8 94375-81-2 94676-99-0 95220-02-3

96579-26-9 101635-19-2 114697-01-7 115097-86-4

IT 96579-26-9

RN 96579-26-9 CAOLD

Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) CN

(CA INDEX NAME)

ACNH OAC $AcO-CH_2-CH-CH-CH-CH-CH-(CH_2)_{12}-Me$

L33 ANSWER 12 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA51:4272c CAOLD

TITLE:

sphingolipide series - (IV) detn. of the configuration of

the amino C atom in sphingosine

AUTHOR NAME: INDEX TERM:

Prostenik, M.; Munk-Weinert, M.; Sunko, D. E. 13552-54-0 16538-04-8 26547-18-2 **96579-26-9**

103043-32-9 103043-93-2 103044-19-5 103044-86-6 103045-14-3

103047-85-4 122389-37-1

IT 96579-26-9

RN 96579-26-9 CAOLD

CN Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI)

(CA INDEX NAME)

AcNH OAc

L33 ANSWER 13 OF 13 CAOLD COPYRIGHT 2000 ACS

ACCESSION NUMBER: CA51:1035h CAOLD

TITLE:

cyclic sulfites derived from the chloropropanediols

AUTHOR NAME:

De la Mare, P. B. D.; Klyne, W.; Millen, D. J.; Pritchard,

J. G.; Watson, D.

INDEX TERM:

497-04-1 1469-73-4 96-24-2

4176-55-0 3741-38-6

4176-57-2 15121-11-6 **96579-26-9** 122330-92-1

ΙT 96579-26-9

RN 96579-26-9 CAOLD

Acetamide, N-[2-(acetyloxy)-1-[(acetyloxy)methyl]-3-heptadecenyl]- (9CI) CN

(CA INDEX NAME)

AcNH OAc $AcO-CH_2-CH-CH-CH=CH=CH-(CH_2)_{12}-Me$

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